DIESEL FUEL CETANE NUMBER EFFECTS ON ENGINE EFFICIENCY AND EMISSIONS

A Thesis

by

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ABSTRACT

Diesel engine combustion is heavily impacted by the chemical and physical properties of the fuel being used. Fuel composition plays a role in the in-cylinder behavior of the fuel and the emissions produced during combustion. Particularly, the Cetane Number (CN) of the fuel, which quantifies the ignition characteristics of the fuel, significantly impacts the quality and mode of the combustion. In this study, a low CN (30) Fuels for Advanced Combustion Engines (FACE) fuel is blended with two higher CN fuels; a Palm Methyl Ester (PME) biofuel and a Fischer-Tropsch Gas to Liquids (GTL) diesel. The blends are formulated to match the CN of 55 of a high CN FACE fuel. The fuel blends are used to operate a light-duty diesel engine to identify the combustion characteristics of the fuel under a moderate load, approximately 4.5 bar Brake Mean Effective Pressure (BMEP), with high and low levels of Exhaust Gas Recirculation (EGR). To decouple combustion phasing effects within the cycles, the 50% mass fraction burned point is matched for all fuels by adjusting the start of fuel injection timing. The performance of the blended fuels is then compared to the high and low CN FACE fuels. The CN of each fuel is found to be the primary driving factor in the emissions and efficiency achieved. The low CN FACE fuel produced higher NOx emissions and lower combustion efficiency under high and low EGR operation than each of the high CN fuels. The PME and GTL fuel blends produced lower smoke emissions than the high CN FACE fuel under high EGR operation, but slightly higher NOx, CO, and THC emissions under both high and low EGR operation.

DEDICATION

To Chelsea, Taggart, my family, my mentors, and my friends.

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I would like to primarily thank my wife, Chelsea, for being my best friend, my inspiration, my sounding board, my biggest supporter, and my late-night coffee barista. Thank you for giving me your support and pushing me to be better every day. I cannot wait to see what the future holds for us.

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NOMENCLATURE

EGR	Exhaust Gas Recirculation
PCCI	Pre-mixed Charge Compression Ignition
HCCI	Homogenous Charge Compression Ignition
RCCI	Reactivity Controlled Compression Ignition
CI	Compression Ignition
MAF	Mass Air Flow
CAD	Crank Angle Degree
RPM	Revolutions per Minute
TDC	Top Dead Center
BTDC	Before Top Dead Center
ATDC	After Top Dead Center
CA10	10% Mass Fraction Burned Crank Angle
CA50	50% Mass Fraction Burned Crank Angle
CN	Cetane Number
T90	90% Distillation Temperature
SOI	Start of Injection
MAF	Mass Air Flow
BMEP	Brake Mean Effective Pressure
BSNOx	Brake Specific Oxides of Nitrogen
BSFC	Brake Specific Fuel Consumption
BFCE	Brake Fuel Conversion Efficiency

NOx	Oxides of Nitrogen
CO	Carbon Monoxide
CO_2	Carbon Dioxide
O_2	Oxygen
THC	Total Hydrocarbon
PM	Particulate Matter
FSN	Filter Smoke Number
FID	Flame Ionization Detection
NDIR	Non-Dispersive Infrared
DC	Direct Current
PME	Palm Oil Methyl Ester
FAME	Fatty Acid Methyl Ester
GTL	Gas to Liquids
FACE	Fuels for Advanced Combustion Engines
HRR	Heat Release Rate

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1. INTRODUCTION

1.1. Motivation

Diesel engines are the prime movers of the world economy, and no viable alternatives exist at the moment to replace them on a large scale. As such, there is an ever-increasing demand to operate diesel engines in a more efficient and inexpensive manner. While research into new and improved engine designs is ongoing, and developments such as Pre-mixed Charge Compression Ignition (PCCI), Homogenous Charge Compression Ignition (HCCI), and Reactivity Controlled Compression Ignition (RCCI) engines show promise for the future of compression ignition (CI) engines, there is a need to improve the operation of existing engine systems [1]. The use of higher quality, intelligently designed fuels provides a gateway to improving the emissions and efficiency achieved by existing engine systems.

The rising cost of fuel and the need to decrease greenhouse gas emissions have driven interest in exploring methods to improve the quality of combustion achieved by diesel engines. The drawback of using inexpensive, lower quality, diesel fuels is that they can produce high levels of many harmful emissions, particularly PM and NOx, and it can be difficult to optimize engine performance for such fuels [2]. Numerous studies have been undertaken to develop methods to improve the combustion characteristics of diesel fuels through the use of various blends and additives [3-5]. Of note, biofuels such as Palm Methyl Ester (PME) and synthetic fuels such as Fischer-Tropsch Gas-to-Liquid (GTL) diesel have shown promise for improving the combustion properties of base diesel fuels [4-7]. This study has been undertaken in order to study the effects of drastically changing fuel chemistry and the physical makeup of a fuel whilst holding the cetane number constant.

1.2. Background

Diesel engines are CI engines relying on the compression of the cylinder contents, and the injection of fuel into the cylinder at the correct time to produce a combustible mixture and ignite the fuel-air mixture [2]. Several variables affect the combustion process that occurs in a CI engine including the properties of the fuel, the combustion chamber design, the injection strategy (duration, timing, pressure, pattern, etc.), the engine speed, and the applied load [2]. The fuel must flow through the fuel injector, atomize, mix with the air in the cylinder, and ignite at the proper time in the cycle in order to fully combust and produce the lowest possible amount of harmful emissions. Because the combustion of a fuel in a CI engine has no external ignition source, the fuel must have properties that are favorable for auto-ignition under the desired conditions.

The primary means of quantifying the auto-ignition characteristics of a diesel fuel is the cetane number, or CN [8]. The higher that the CN of a fuel is, the shorter delay that will occur between injection and ignition of the mixture. The CN of a fuel is a measured quantity, and encompasses data about the physical properties and the chemical volatility of the fuel. The ignition delay for a diesel fuel is defined commonly and in this study as the time from the start of injection to the beginning of the main heat release, the 10% fuel mass fraction burned, or CA10 location [2, 8]. This ignition delay is important because it has profound impacts on the combustion process that will occur in an engine, and is a driving factor in the balance between diffusion and pre-mixed combustion in the cylinder.

The longer the ignition delay, the more pre-mixed the air-fuel mixture in the cylinder will become, thus leading to high amounts of pre-mixed combustion, , and lower amounts of diffusion burn [9]. Diffusion burn within the cylinder is primarily responsible for PM emissions,

whereas the pre-mixed burn portion is typically responsible for the NOx emissions due to the high in-cylinder temperatures [2, 10]. The emissions produced by a diesel engine are heavily dependent on the timing, type, and quality of combustion, so fine control of the combustion process is desired.

1.3. Objective

The objective of this study is to assess the impacts on emissions and efficiency of altering fuel chemistry and physical properties while holding CN constant.

The Fuels for Advanced Combustion Engines (FACE) fuel program was created to allow for the testing and observation of diesel fuels at different design points [11]. FACE fuels were chosen for this study because of their known physical and chemical characteristics.

In this study, the FACE 1 fuel (CN of 30) and FACE 5 fuel (CN of 55) are used. Each FACE fuel used has the same T90 distillation temperature of 270° C and 20% aromatic content. The FACE 1 fuel is used as the base fuel that will be blended with a high CN PME biofuel and a high CN GTL fuel. The fuels will be tested using realistic steady-state operating conditions for a light-duty diesel engine under a medium load with both high and low Exhaust Gas Recirculation (EGR) rates. The objective of this study is to examine the emissions and efficiency effects of increasing CN by drastically varying fuel composition using the PME and GTL fuel blends.

2. LITERATURE REVIEW

2.1. Overview

In his original 1895 patent entitled *Method of and Apparatus for Converting Heat Into Work,* Rudolf Diesel referenced the importance of the properties, particularly what he called the "Ignition Point" of a specific fuel with regards to its performance in his apparatus [12]. Diesel speaks to the behavior of a fuel introduced into a high-pressure, high-temperature environment as a determining factor in the work produced by the engine [12]. Over the ensuing century, countless studies and patents have been filed regarding new and improved methods of formulating fuels for use in diesel engines. Considerable research has been conducted in order to develop methods to improve the combustion characteristics of diesel fuels, including work dedicated to the study of each fuel constituent utilized in this experiment [6, 7, 11, 13-18]. The work conducted by Li examined the effects of each fuel parameter controlled by the FACE fuel matrix on engines of different sizes, under different load conditions [19]. An alternative approach is taken in this study in order to examine the effects of drastically different fuels on the same light-duty engine utilized by Li.

The following literature review will examine the background of this research and the fuels utilized, as well as the fundamental mechanisms behind the crucial emissions parameters being studied.

2.2. Fuel Properties

Extensive research has gone into discovering and identifying the critical fuel parameters that are driving factors in the performance of a fuel in a diesel engine. Studies conducted by

Mueller et al. utilized FACE fuels to characterize the fuel components and their effects on combustion in hopes of producing surrogate fuels to match target fuels to be used in advanced combustion technique research [20, 21]. Li et al. utilized the full matrix of FACE fuels to characterize the effects of CN on the combustion effects between different sizes of engines, and found that the engines become more sensitive to CN as load increases, and that the engine size can have a large effect on the sensitivity to CN [19, 22]. Fuel research conducted by Westerholm and Egebäck found that the most important diesel fuel parameters related to the engine-out emissions were the polycyclic aromatic hydrocarbon (PAH) content, aromatic content, T90, final boiling point, specific heat, density, and sulfur content [23]. In order to properly identify the differences in combustion and behavior between fuels, these parameters must be addressed. The standards for testing and characterizing fuel parameters are contained in American Society for Testing and Materials (ASTM) standard specifications [24].

2.2.1. Cetane Number

The CN of a diesel fuel is an indication of the ignition characteristics of the fuel. The primary fuel behavior quantified by the CN is ignition delay, which is determined by a number of factors, including physical and chemical properties. The fuel fluid properties of density, viscosity, vaporization temperature and rate, and surface tension affect the physical delay in the ignition process, and the chemical structure of the fuel determines any chemical delay in ignition [25]. The ignition process of a hydrocarbon fuel and the properties which affect the ignition process are presented by Murphy et al. in Figure 1 [25] :.

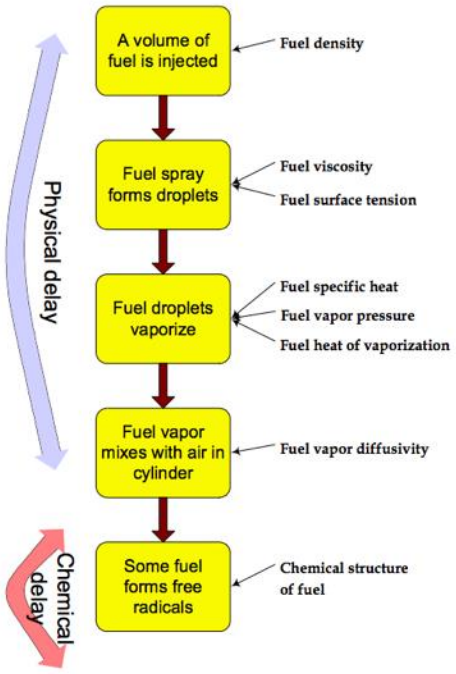

Figure 1 - Fuel Ignition Process, reproduced from [25]

While CN is widely accepted as the standard for quantifying the ignition quality of a fuel, there have been concerns in the past regarding its applicability to alternative fuels that have different properties than traditional fossil-fuel middle-distillate fuels [26, 27]. The reported CN of a fuel can often vary considerably depending on the process and means of testing [25]. Issues arise in the calculation of CN values for fuels that have been blended with other diesel fuels. Typically, the calculated CN can be assumed to be linear based on blending rules, however there may also be non-linear effects on the CN that are not accounted for [25]. The concerns regarding the accuracy of CN measurements for various fuels has driven research into accurately measuring and quantifying the ignition quality of fuels. The use of concepts such as derived cetane number (DCN), and technologies such as the Ignition Quality Tester (IQT) allow for the

more rapid measurement of a fuel's ignition characteristics, and show promise for accurately reporting data for alternative fuels [28, 29].

2.3. FACE Fuels

In hopes of achieving a baseline for fuel research to work from, the Advanced Vehicle/Fuel/Lubricant (AVFL) working group within the Coordinated Research Council (CRC) developed the FACE working group and fuel program in 2006 [11, 30]. Dr. Brad Zigler of the National Renewable Energy Laboratory (NREL) presented the objective of the FACE working group: "To develop, characterize, and recommend research fuel sets that can be used broadly in research efforts to provide tie-points between these efforts that will further increase the understanding of fuel property impacts on advanced combustion processes, their efficiency, and their emissions" [30]. The FACE working group developed a fuel matrix for both diesel and gasoline fuels [30]. The FACE diesel fuel program focused on designing fuels that controlled for ignition quality (CN), chemistry (aromatic content), and volatility (T90) [11]. The FACE fuel design matrix contains nine fuels, the design parameters of which are shown in Figure 2.

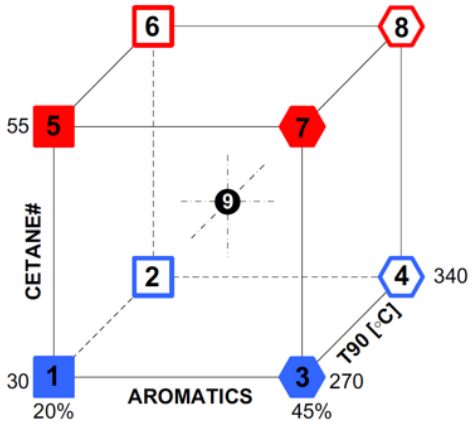

Figure 2 - FACE Fuel Design Matrix, reproduced from [11]

The FACE diesel fuel matrix was designed to give two levels of the three important design criteria to study, a CN ranging from 30 to 55, T90 ranging from 270°C to 340°C, and an aromatic content ranging from 20% to 45% [18]. The design criteria for the FACE fuel 9 was chosen to be in the center of the matrix: a CN of 42.5, T90 of 305° C, and an aromatic content of 32.5% [18]. All of the FACE fuels were designed to have less than 15 ppm of sulfur, and less than 4% olefin content by volume [18].

The FACE fuel matrix has been used by a number of studies as a means of analyzing the behavior and operation of novel engine operating techniques such as HCCI, PCCI, and RCCI [31-34]. Anand et al. conducted a study to establish proper surrogate fuel models to replicate the combustion characteristics of each FACE fuel within a maximum error of 4%, which allows for the use of the fuel models in computational fluid dynamics (CFD) simulations [35]. The FACE fuels 1 and 5 were chosen as baseline fuels for this study.

2.4. PME Biofuel

Palm Methyl Ester (PME) is a Fatty Acid Methyl Ester (FAME) biofuel produced from palm oil, which has gone through the process of transesterification [17]. The PME fuel used in this study is sourced from Shell Global Solutions. Figure 3 - PME Production Processprovides a graphic description of PME production.

Figure 3 - PME Production Process

Transesterification involves reacting an oil with an alcohol, typically methanol or ethanol and a catalyst in order to generate fatty acid methyl esters and glycerol [36]. ASTM standard D6751 outlines the standard specifications for the production of biodiesel [37].

A main draw of biofuels in general is that they can be utilized with little or no modification to the existing engine systems, and biofuels typically produce fewer harmful emissions [16]. Ng et al. conducted a study to establish a characterization of the engine responses to varying levels of PME blended with an equally high CN fossil diesel. Increasing the PME concentration in this study was found to decrease the PM and THC emissions out of the engine for a given speed and load [16]. Lapuerta et al. concluded that there is a wide disparity in the reported emissions and efficiencies reported while utilizing biofuels due to the wide differences in fuel properties between biofuels [38]. However, the majority of studies report decreases in PM, CO, and THC emissions when utilizing a biodiesel blend or neat biofuel [16, 38].

While biofuels can have benefits in regards to emissions, they typically are documented to have higher BSFC due to lower heating values as compared to conventional diesel [39]. PME has higher oxygen content than conventional diesel, lower sulfur content, and no aromatics [39].

PME biofuel's density can range from 860-900 kg/m^3 and the kinematic viscosity ranges from 3.5-5.0 mm^2/s [40]. Biofuels have higher viscosity and density than conventional diesel, so the spray atomization quality is not as high as lower viscosity diesel fuels [39]. This viscosity difference also plays a role in biofuels' applicability in colder climates [41].

2.5. GTL Diesel Fuel

GTL diesel fuel is a synthetic diesel fuel produced from natural gas using the Fischer-Tropsch (FT) method. GTL is often referred to as FT diesel in the literature [7]. The GTL diesel used in this study is sourced from Shell Global Solutions. GTL diesel is produced by converting natural gas to a liquid hydrocarbon diesel fuel through the FT process. GTL diesel typically has better ignition characteristics than conventional diesel fuels, and can be implemented in both neat fuel form and as an additive to conventional, lower quality diesel fuels.

2.5.1. Fischer-Tropsch Method

FT fuels can be produced from a number of carbon-based materials including coal, natural gas, and biomass [7, 42]. Figure 4 – Fischer-Tropsch Processprovides a graphical representation of the Fischer-Tropsch Method.

Figure 4 – Fischer-Tropsch Process

The FT process involves producing hydrocarbons from carbon monoxide and hydrogen, called synthesis-gas, that are cracked from the base carbonous material [7, 43, 44]. The feed-stock materials are partially oxidized in order to create synthesis-gas, then the synthesis-gas components are recombined into larger hydrocarbon molecules, which are then post-processed into a number of different materials including fuels, lubricants, and waxes [6, 43, 44]. FT fuels are classified into two categories depending on the temperature at which the recombination of the CO and H2 occurs: low temperature (200-240°C), which utilizes an iron-based catalyst for synthesis, and high temperature (300-350°C), which uses either an iron or cobalt-based catalyst [7]. The FT process can be modified, primarily in the post-processing, to produce specifically designed products, such as fuels with better lubricity or cold-flow properties [7, 43].

2.5.2. Fuel Properties

Typically, GTL diesel is created using a low-temperature FT process, which yields diesels with very low, or zero aromatics, near-zero sulfur content, and high CN values of 70 or greater [7, 43, 44]. Wu et al. found that GTL densities were typically 7.2% lower than that of conventional diesel, with similar viscosity [5]. The density of GTL diesel fuel is approximately 790 kg/m^3, and the kinematic viscosity is approximately 3 mm^2/s [45]. In studies utilizing a high-CN GTL diesel, it is typically found that due to GTL diesel's high CN and low aromatic content, the emissions produced from combustion are typically preferable to the products of conventional diesel combustion [7, 13, 44, 46]. The improvement in NOx formation seen when utilizing a GTL diesel fuel in either neat or blended formats can typically be attributed to the improvement in CN over a conventional diesel fuel [13]. GTL diesels with low distillation temperatures also display reduced PM emissions over conventional diesel fuels [13]. Overall,

there are clear emissions benefits from introducing GTL fuels, both in neat forms and as an additive to improve the properties of base diesel fuels [44].

2.6. NOx Emissions

The formation of oxides of nitrogen, or NOx, is crucially important in diesel engine combustion research. NOx is the nomenclature accepted to describe emissions of NO and NO_2. The formation of NO is described by the extended Zeldovich mechanism [2, 47-49]. The extended Zeldovich mechanism presents the equilibrium equations governing the creation and destruction of NO [2].

$$O + N_2 = NO + N \quad (1)$$

$$N + O_2 = NO + O \quad (2)$$

$$N + OH = NO + H \quad (3)$$

The second constituent of NOx, NO_2 makes up 10 to 30 percent of the NOx in the emissions of diesel engines, with the NO/NO_2 ratio heavily depending on engine speed and load [2]. NOx formation is heavily dependent on the temperatures achieved in the cylinder during combustion. Typically, higher levels of pre-mixed burning in the cylinder lead to high in-cylinder temperatures. Of particular importance in this study, a fuel with a longer ignition delay (lower CN) will produce more NOx during combustion. NOx can also be strongly controlled by the introduction of EGR into the cycle due to the lower peak in-cylinder temperatures achieved during combustion [2].

2.7. PM Emissions

PM emissions are often referred to in a number of ways, whether particulates, smoke, or soot. The reason behind this variance in definition is that PM is difficult to specifically classify. PM emissions are solid carbon particles that are formed from unburned fuel [50, 51]. Tree et al. describes the soot formation process into six independent phases: pyrolysis, nucleation, coalescence, surface growth, agglomeration, and oxidation [50]. A useful soot formation schematic is reproduced from in Figure 5 [50].

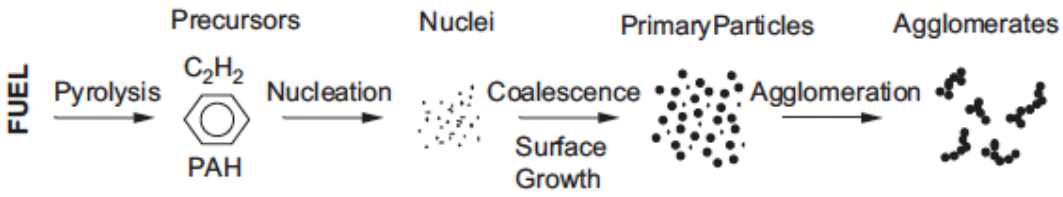

Figure 5 - Soot Formation Process, reproduced from [50]

A number of factors influence the PM formation process in a combustion event. Namely, the temperature, pressure, equivalence ratio, fuel properties, and injection strategy [50]. The influence of fuel properties on PM formation has been extensively studied, including studies utilizing biofuels and FT diesel fuels [46, 52]. In this study specifically, the smoke emissions are measured by Filter Smoke Number (FSN).

3. EXPERIMENTAL METHODOLOGY

3.1. Engine Control and Measurement

3.1.1. Engine

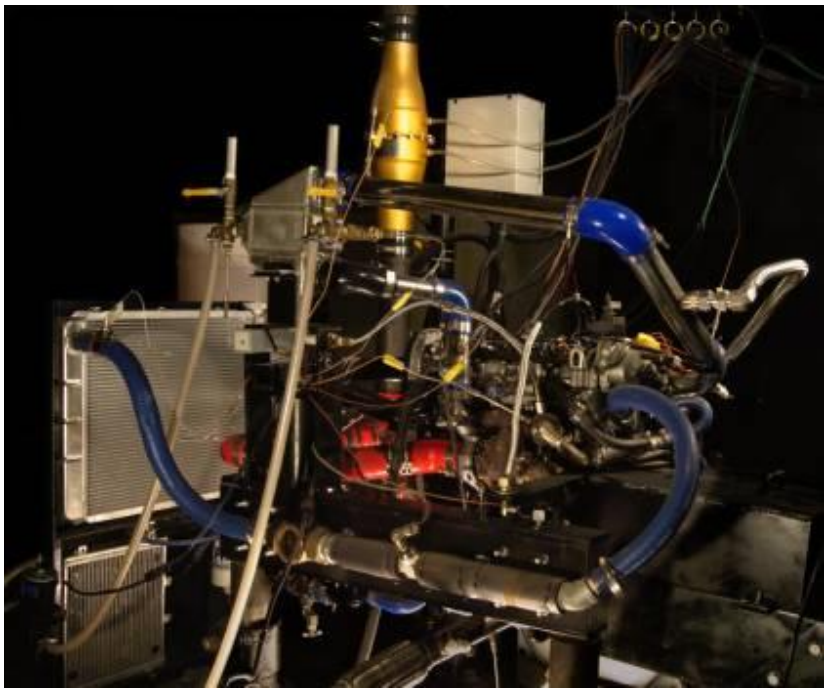

Figure 6 - Light-duty 1.9 L Diesel Engine

The engine used in this study is a General Motors four-cylinder light-duty direct injection CI engine with a high-pressure common rail fuel system, a variable geometry turbocharger and a cooled EGR loop. The engine is presented in Figure 6. The design specifications for the test engine are listed in Table 1.

Parameter	Design Specification
Displacement	1.9 L
Stroke	90.4 mm
Bore	82 mm
Compression Ratio	18:1 (nominal)
Rated Power	110 kW at 4000 RPM
Rated Torque	315 N-m at 2000-2750 RPM

Table 1 - Test Engine Geometric Design Specifications

The engine is outfitted with a two-stage low-pressure fuel supply system and a belt-driven high-pressure fuel pump feeding a common rail supplying electronically controlled fuel injectors. The low-pressure fuel supply system includes positive displacement flowmeters to calculate the exact mass flow of fuel being supplied to the cylinders on a kilogram per hour basis. The flow of fuel into the cylinders is controlled by varying the common rail pressure and the fuel injection duration into the cylinder. The EGR loop includes a valve that can be manipulated to control the flow of EGR into the intake manifold; this valve allows fine control of the mass of fresh air into the engine. The variable-geometry turbocharger on the engine allows for control of the intake manifold pressure. The mass-airflow sensor on the engine accurately measures the total mass of fresh air flowing into the intake manifold from the compressor side of the turbocharger in a kilogram per hour basis. This fine control of fuel and air allows for the accurate control of the fuel-air ratio for a given test condition, as will be discussed further in the experimental methodology section.

3.1.2. Controller

Engine operation is controlled by a third-party control software developed on a LabVIEW framework. The control system allows for the measurement and control of numerous engine parameters. Integrated into the control software is a high-speed data acquisition system, which records and averages data over 200 engine operating cycles.

3.1.3. Engine Control

Of note, the control system allows the common rail fuel pressure and the fuel injection events to be specified, both in timing and duration. Through the manipulation of the EGR valve, the intake MAF can be controlled. The engine speed is controlled by a DC electric motoring dynamometer, and engine load is controlled by the fuel delivery into the cylinders.

3.1.4. Parameter Measurement

Engine operating parameters such as coolant temperatures, and intake and exhaust temperatures and pressures are measured using both stock and auxiliary sensors interfaced with the control system. The information is translated by the control software and produced in a usable form during data recording.

Each cylinder on the engine is equipped with a piezoelectric pressure transducer that allows for the rapid measurement of in-cylinder pressure throughout the operating cycle. The engine is equipped with an encoder that allows the pressure measurements to be correlated to the crankshaft position on a resolution of 0.2 CAD. The in-cylinder pressure traces allow for observation of the combustion process.

3.1.5. Emissions Measurement

Exhaust emissions data is recorded by a Horiba Mexa 7100D emissions bench, which measures the following emission species: NOx emissions by heated chemiluminescence, CO and CO_2 emissions by NDIR, THC emissions are measured by FID, and O_2 is detected by a magneto-pneumatic analyzer [53-56].

NOx measurement by chemiluminescence is an industry accepted standard for quantifying NOx emissions. Chemiluminescence is the emission of light from a molecule involved in a chemical reaction [57]. As NO particles enter the analyzer, they are reacted to form NO_2 and emit light. In addition, as NO_2 particles enter the analyzer, they are dissociated to NO, and then routed through the chemiluminescence analyzer [54]. Virtually all of the NOx particles leaving the analyzer have been converted to NO_2 after analysis.

Analysis of the CO and CO_2 components of the engine emissions is completed by the optical method of NDIR [56]. As particles enter the analyzer, infrared light is transmitted through the sample. The different molecules absorb the infrared light at different rates, and the level of absorption is directly correlated to the concentration of specific molecules such as CO or CO_2 [56]. The Mexa 7100D has two separate NDIR sensors which are calibrated to analyze CO and CO_2 individually.

Hydrocarbon emissions are measured by a FID analyzer in the Mexa 7100D. The hydrocarbon emissions are combusted in the analyzer. As the hydrocarbons are burned, there is a small flow of ions from the flame that can be detected by the FID. This flow of ions is proportional to the carbon atoms that are in the THC emissions [56]. The THC emissions are reported in terms of carbon atoms.

Oxygen emissions are measured by the magneto-pneumatic analyzer. The magneto-pneumatic analyzer works on the principle that if a paramagnetic gas is subjected to a strong enough magnetic field, the pressure in the immediate area will increase proportionally. Alternating magnetic fields provide an accurate measurement of the oxygen content of the sample [58]. The Mexa analyzer is presented in Figure 7.

Prior to each testing day, the emissions equipment is calibrated and spanned to match known gas concentrations for each emissions species to ensure proper measurement reliability and decrease uncertainty.

Figure 7 - Horiba Emissions Analyzer

The emissions data measured by the Horiba emissions bench is transmitted directly to the control and data acquisition system. In this study, PM emissions are not measured. Instead, smoke emissions are measured by an AVL smokemeter, which reports smoke emissions as FSN, an optical measure of opacity of a filter paper. The smoke meter data is recorded using a secondary computer system separate from the main control and data acquisition system.

3.2. Fuel Matrix

The fuels used in this study are specially formulated and blended to achieve the goal of matching CN while varying the fuel composition. A blend matrix of five fuels was devised. Table 2 presents the fuel blends and their calculated or known CN. Commercially available Diesel #2 was used as a baseline comparison fuel for testing. The base fuel components used in this study are the FACE fuels one and five, which correspond to the low CN, low aromatic content, low T90, and the high CN, low aromatic content, low T90 fuels respectively [30]. The fuel components being blended into the low CN FACE 1 fuel are Shell PME biodiesel, which has a CN of 70 and Shell GTL diesel, which has a CN of 80.

Fuel	Component 1 (Volume %)	Component 2 (Volume %)	CN	Density (kg/m^3)
1	#2 Diesel – 100%	N/A	51	826
2	FACE 1 – 100%	N/A	30	828
3	FACE 1 – 34%	PME – 66%	55	860
4	FACE 1 – 44%	GTL – 56%	55	804
5	FACE 5 – 100%	N/A	55	806

Table 2 - Fuel Blend Matrix

The PME fuel and the GTL fuel were provided by Shell Global Solutions in neat form, and the FACE fuels were manufactured by Haltermann Solutions. Fuel blending was performed in house as a part of the study. Tests of the study fuels performed by the Shell Global Solutions fuels lab confirmed that blending the high CN PME and GTL fuels into the low CN FACE 1 fuel produced blended fuels with the target CN value of 55.

3.3. Test Conditions

3.3.1. Baseline Testing

Baseline testing was performed using commercial Diesel #2 to establish appropriate test conditions for the fuel blends. In order to analyze the differences in the fuels, the combustion process needs to be stressed by introducing EGR and or increasing load. It was established through the baseline testing that the fuels should be tested at two steady air-fuel equivalence ratios by varying the amount of EGR that flows into the intake manifold. The fueling rate (determined by common rail pressure and injection duration) is held constant for all test conditions.

3.3.2. Combustion Phasing

Combustion phasing within the engine's cycle has a large effect on the quality and type of combustion that occurs; thus, the combustion phasing needs to be consistent across all test fuels. The parameter used in this study to align combustion phasing is CA50. In this study, the test fuel's CN, the engine speed, the injection duration, the level of EGR, and the SOI are the determining factors in the CA50 location in the cycle. The effect of CN on combustion phasing as referenced by Szybist et al. highlights the necessity for the CA50 locations to be appropriately

matched across all test fuels [59]. Combustion phasing will be matched by calibrating injection timing during the baseline testing to match CA50 location. For Diesel #2 at the desired operating conditions, the CA50 location is at approximately 11.5 °ATDC, which was chosen as the target CA50 for the study fuels. As the test fuels and level of EGR are changed, the SOI for each fuel will be adjusted from the initial test matrix to achieve a CA50 location within 1 CAD of the target.

3.3.3. Fuel Metering

Ideally, the mass of fuel delivered into the cylinder during each test condition would be adjusted such that the same amount of fuel energy is delivered to the cylinder across all test fuels. However, due to the nature of the mechanical high-pressure fuel pump, and the resolution available in the fuel delivery measurement, the precise control necessary to achieve that goal is not possible with this apparatus. Instead, the fuel injection duration is held constant across all fuels. Slight differences in the exact fuel quantity delivered are due to the inherent uncertainty of the fuel delivery system and slight differences in fuel properties. When conducting baseline testing with Diesel #2 with a common rail pressure of 900 Bar, and an injection duration of 0.60 ms, the target fuel mass flowrate is 2.6 kg/hr. This fuel injection strategy produced an engine loads appropriate for testing the fuel blends, and allowed for the introduction of high EGR without creating very high levels of CO, THC, and FSN emissions.

3.3.4. EGR Setting

The amount of EGR that is introduced into the intake manifold is controlled by the MAF setting within the control software, which adjusts the EGR valve on the engine. During the

baseline testing, it was found that holding a specific MAF set-point within the control software produced constant EGR rates. With the target EGR rates, the chosen MAF values produced test condition equivalence ratios equal to 0.43 for low EGR and 0.63 for high EGR. Due to the nature of this study, fueling and airflow will remain constant across all test fuels in order to maintain constant equivalence ratios at the two EGR rates.

3.3.5. Baseline Test Matrix

Table 3 outlines the initial operating conditions that were deemed appropriate during baseline testing. All testing is completed with a fuel rail pressure of 900 bar.

Fuel	Injection Duration (ms)	Injection Timing (°BTDC)	MAF (kg/hr)	Target EGR %
1	0.60	0	90	15
1	0.60	1	60	30
2	0.60	0	90	15
2	0.60	1	60	30
3	0.60	0	90	15
3	0.60	1	60	30
4	0.60	0	90	15
4	0.60	1	60	30
5	0.60	0	90	15
5	0.60	1	60	30

Table 3 - Proposed Operating Condition Test Matrix

3.4. Experimental Procedure

3.4.1. Fuel Blend Management

Figure 8 - Fuel Blend Process

Each of the test fuels are blended into clean empty fuel containers, and each fuel has its own supply line with an in-line filter and a quick disconnect fitting to properly interface with the existing low-pressure fuel supply system. The design of the fuel system on the test engine requires a special procedure in order to properly purge the existing fuel in the lines prior to testing with the fuel blends. This procedure must be completed before each test fuel can be run through the engine in order to remove the possibility of cross contamination of the fuels. The fuel blend process is seen in Figure 8.

Before testing each fuel, the supply line of the low-pressure fuel system is connected to the test fuel, and the return line is placed in a waste container. The low-pressure system is then purged for an appropriate amount of time into the waste container. The time needed to purge the low-pressure supply system was determined based on the steady flow rate from the low-pressure pump and a conservative estimate of the system volume. After purging, the return line is placed back into the test fuel container. This procedure prepares the low-pressure system to be operated as a part of the engine test apparatus.

3.4.2. Setting Injection Timing

Prior to collecting data, the engine is operated at the desired test condition for approximately 30 minutes and brought to steady state as determined by the exhaust manifold temperature. Once the exhaust manifold temperature has reached a steady state, the SOI needs to be adjusted for each fuel in order to match the desired CA50 location of 11.5° BTDC. Each fuel is tested using a constant fuel injection strategy, so the changing fuel properties, particularly CN, require that the fuel SOI for each test condition be calibrated to the fuel being used.

3.5. Final Test Matrix

Upon measuring the appropriate SOI for each fuel in order to match CA50, the corrected test matrix for the study is produced. The final test matrix is shown in Table 4. All testing will occur at 900 bar common rail pressure and 1500 RPM.

Fuel	Injection Duration (ms)	Injection Timing (°BTDC)	MAF (kg/hr)	Target EGR %
1	0.60	0	90	15
1	0.60	1	60	30
2	0.60	1.5	90	15
2	0.60	4	60	30
3	0.60	0	90	15
3	0.60	2	60	30
4	0.60	0	90	15
4	0.60	2	60	30
5	0.60	0	90	15
5	0.60	2	60	30

Table 4 - Final Test Matrix

3.6. Experimental Objectives

The experimental objectives of this study are to collect and analyze the emissions and efficiency data for each test fuel. The analysis will include the Brake Specific NOx (BSNOx) produced, the Brake Specific Fuel Consumption (BSFC), the FSN, and the other major exhaust emissions species of CO, CO2, THC, FSN, and O2. The emissions and fuel consumption data will allow for examination of the efficiencies achieved while the engine is operating on each of the test fuels.

3.7. Calculations

The data recorded by and transmitted to the control system allows for other parameters and information about the engine operation to be calculated. The primary calculated values of concern are the Heat Release Rate (HRR) trace and the EGR rate calculation. The HRR trace is calculated by the method described by Heywood [2] using the in-cylinder pressure measurements and the encoder data. The EGR rate is calculated by measuring the intake and exhaust CO_2. Calculations are further described in this section.

3.7.1. Heat Release Rate

The HRR of the combustion process is calculated in the control software using the method described by Heywood [2]:

$$\frac{\delta Q_n}{dt} = \frac{\gamma}{\gamma - 1} p \frac{dV}{dt} + \frac{1}{\gamma - 1} V \frac{dp}{dt} \qquad (4)$$

Where Q_n is the net heat release from the fuel in the cylinder, γ is the ratio of specific heats, which is assumed to be a constant, p is the in-cylinder pressure, and V is the volume of the combustion chamber [2]. The rate of change of the combustion chamber volume is known from the geometry of the engine, and the rate of change of the pressure in the cylinder is measured by the in-cylinder pressure transducers. The HRR, or $\frac{\delta Q_n}{dt}$, allows for the examination of the timing and mode of combustion that occurs in the cycle.

3.7.2. EGR Fraction

The EGR rate is calculated using the intake and exhaust CO_2 measurements that are made by the Horiba emissions bench. While operating at steady state, the level of CO_2 that is in the intake manifold is measured and entered into the control software. The exhaust CO_2 level is then measured during the data collection to be used to calculated the level of EGR.

$$EGR\ Fraction = \frac{intake\ CO_2\%}{exhaust\ CO_2\%} \quad (4)$$

This calculation was used extensively during the baseline development testing phase to determine the appropriate MAF and fuel flowrates to utilize.

3.7.3. Brake Specific NOx

The NOx emissions in the exhaust are measured in ppm, and that measurement provides an accurate measure of the amount of NOx that an individual operating condition produces. However, because different fuels are being utilized in this study, it is important to adjust the frame in which the NOx emissions are viewed. Because the fuels have different properties, they will invariably maintain slightly different load conditions at the same engine operating settings (fuel flow, MAF, EGR rate). Each fuel will also have different efficiencies, which will all affect the NOx formation. While different fuels and operating conditions may have similar ppm concentrations of NOx, the total NOx emissions can be very different due to efficiency and flowrate changes. Therefore, the appropriate framework for examining the NOx emissions for each cycle is the Brake Specific NOx, or BSNOx.

$$BSNOx = \frac{(\dot{m}_{air} + \dot{m}_{fuel})Y_{NOx}}{\dot{W}_{brake}} * \frac{MW_{NOx}}{MW_{exh}} \quad (5)$$

BSNOx is reported in grams per kilowatt-hour. For the molecular weight of NOx, the molecular weight of NO_2 is used, and the molecular weight of the exhaust is assumed to be equal to the molecular weight of atmospheric air with the addition of the mass of the burned fuel [47].

3.7.4. Brake Specific THC and CO

Similar to the BSNOx calculation, the THC and CO emissions in the exhaust need to be normalized during the data analysis in order to adjust for slight differences in the power output from each fuel.

$$BSTHC = \frac{(\dot{m}_{air} + \dot{m}_{fuel})Y_{THC}}{\dot{W}_{brake}} * \frac{MW_{THC}}{MW_{exh}} \quad (6)$$

$$BSCO = \frac{(\dot{m}_{air} + \dot{m}_{fuel})Y_{CO}}{\dot{W}_{brake}} * \frac{MW_{CO}}{MW_{exh}} \quad (7)$$

The molecular weight of the THC calibration gas, propane, is used in the calculation of BSTHC.

3.8. Uncertainty and Reliability

The test equipment and instrumentation is inspected and calibrated on a regular basis in order to ensure the smallest level of uncertainty in the data collection. Each data point is measured over 200 operating cycles of the engine. Testing with the fuel blends is repeated on a

second day to establish further statistical confidence in the data. The test matrix was randomized between test days to reduce the effect of hysteresis [60]. Furthermore, a long period of development testing using Diesel #2 occurred prior to this study to ensure long-term repeatability and reliability of the test apparatus. The data is analyzed and standard error bars are calculated to a 95% confidence interval using the following equation.

$$Error = \pm\left(\frac{\sigma}{\sqrt{n}}\right) * 1.96 \tag{8}$$

4. RESULTS AND DISCUSSION

4.1. In-Cylinder Pressure and Heat Release Rate

4.1.1. Low EGR

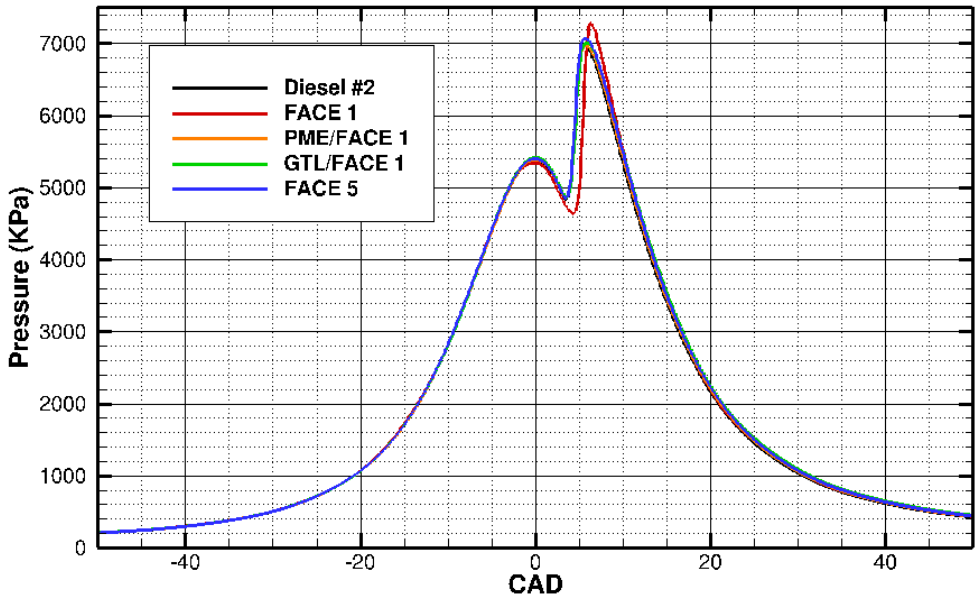

Figure 9 - In-Cylinder Pressure Curves for Low EGR Cases (-50° to 50° ATDC)

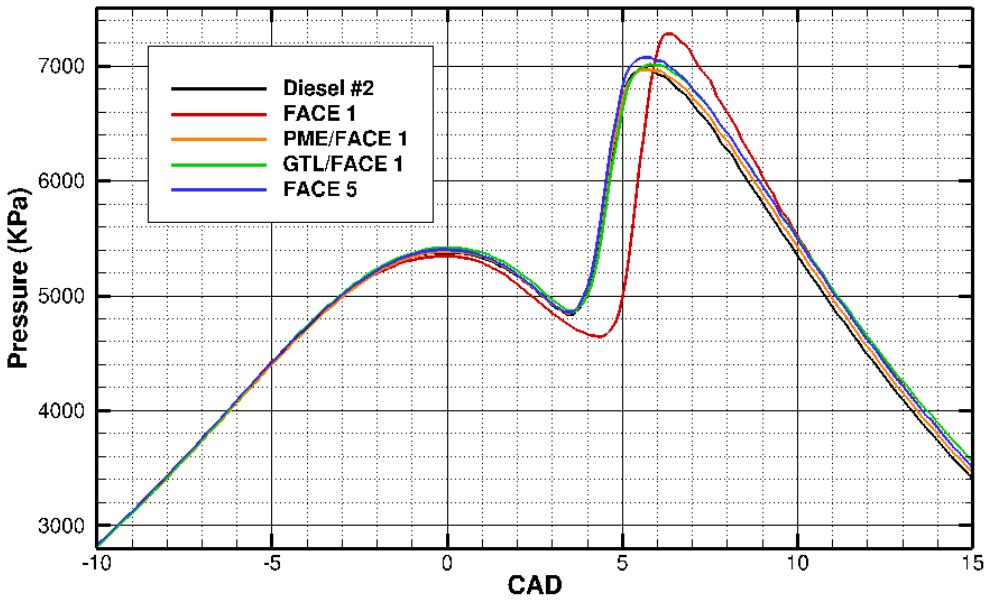

Figure 10 - In-Cylinder Pressure Curves for Low EGR Cases (-10° to 15° ATDC)

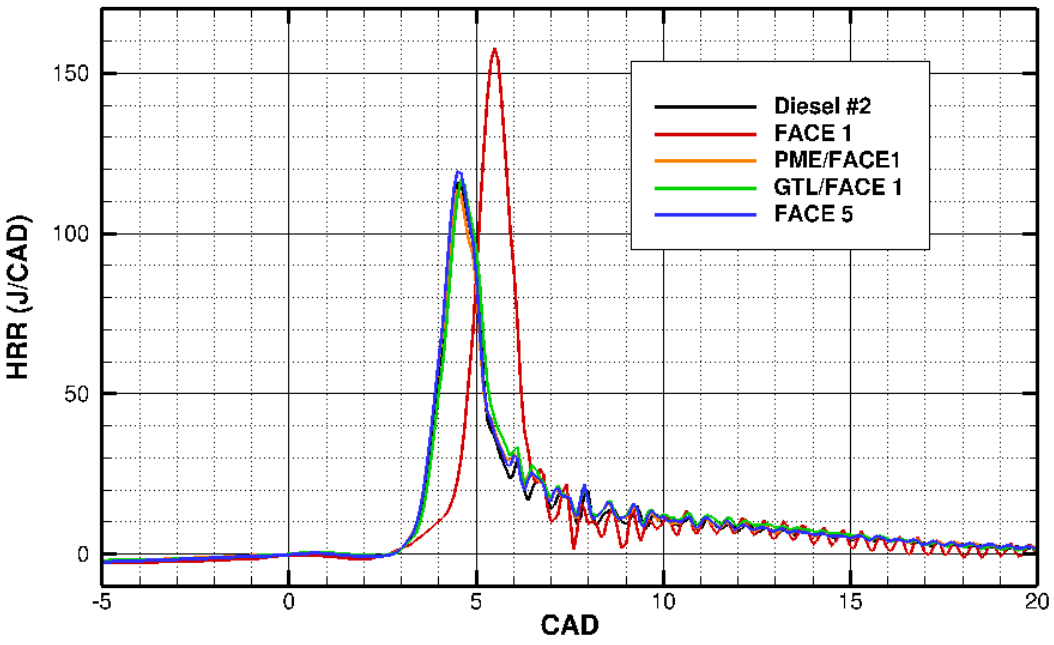

Figure 11 - HRR Plot for Low EGR Cases (-5° to 20° ATDC)

Figure 9 - In-Cylinder Pressure Curves for Low EGR Cases (-50° to 50° ATDC)Figure 10 - In-Cylinder Pressure Curves for Low EGR Cases (-10° to 15° ATDC)and Figure 11 - HRR Plot for Low EGR Cases (-5° to 20° ATDC) present the in-cylinder pressure and HRR for the low EGR cases. In low EGR operation, the high CN fuels, including Diesel #2, all behave similarly in their mode of combustion and pressure rise in the cylinder (Figure 9). Matching CA50 for each of the fuels allows each of the pressure curves to collapse onto each-other. The outlier in the low EGR pressure data is the base FACE 1 fuel with no blend additive (Figure 10). In low EGR operation, the ignition delay of the FACE 1 fuel pushes the peak pressure created to a later point in the cycle, despite the matching of CA50 to within 0.5 CAD.

The low CN FACE 1 fuel exhibits a much higher peak heat release in the HRR curve (Figure 11). The low CN of the FACE 1 fuel allows the fuel to have more time to mix into the air charge in the cylinder. When the FACE 1 fuel reaches the point of ignition, the mode of combustion that occurs is primarily pre-mixed combustion, which leads to the rapid heat release and high peak heat release. The low CN fuel experiences a smaller amount of diffusion burn than the high CN fuels.

4.1.2. High EGR

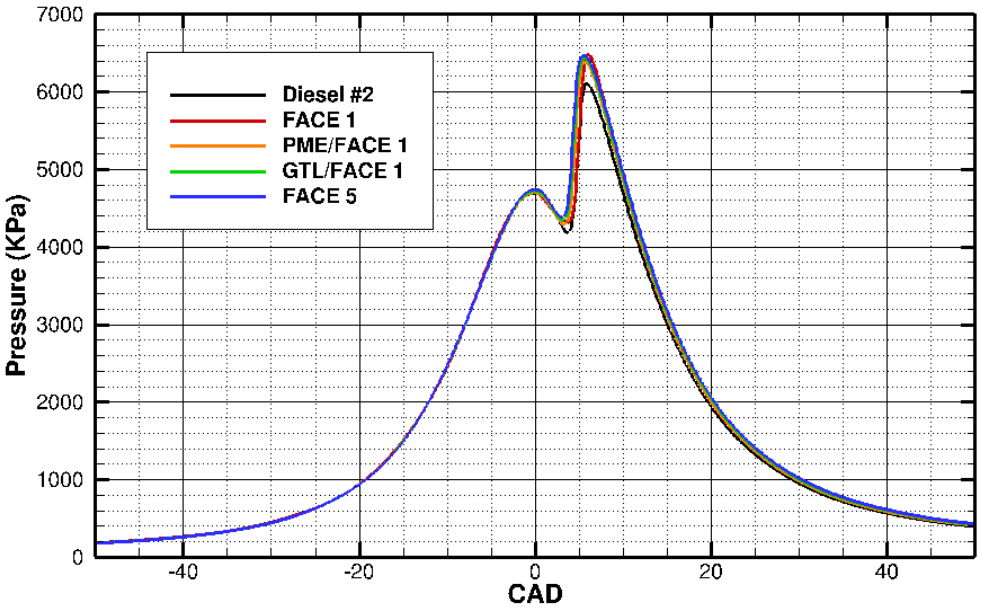

Figure 12 - In-Cylinder Pressure Curves for High EGR Cases (-50° to 50° ATDC)

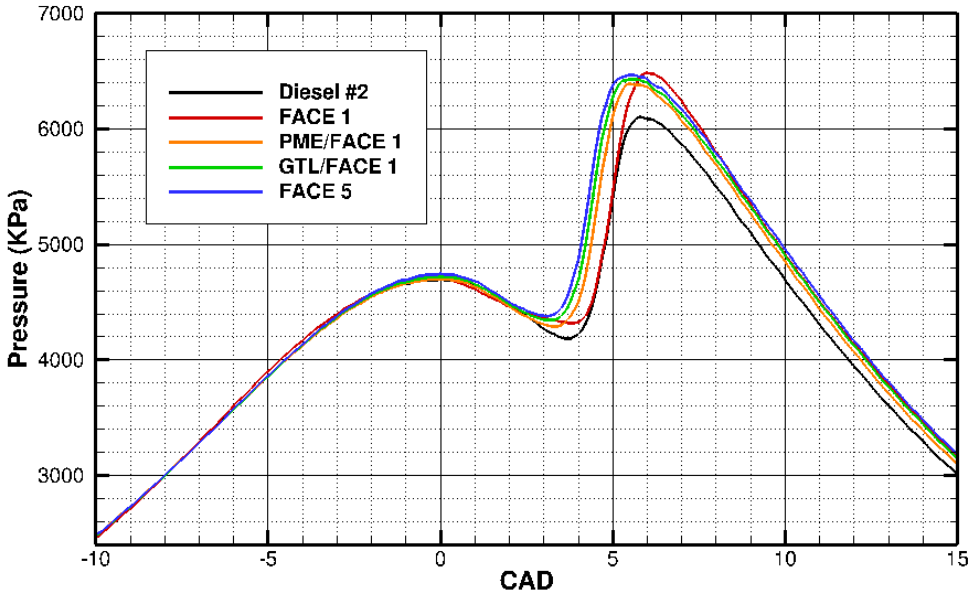

Figure 13 - In-Cylinder Pressure Curves for High EGR Cases (-10° to 15° ATDC)

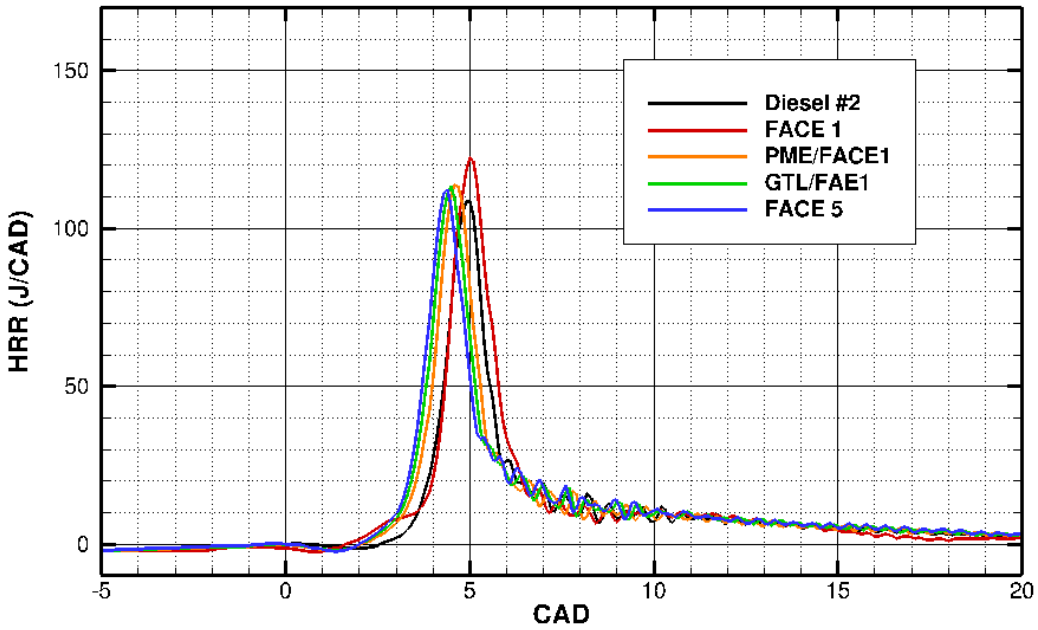

Figure 14 - HRR Plot for High EGR Cases (-5° to 20° ATDC)

Figure 12 - In-Cylinder Pressure Curves for High EGR Cases (-50° to 50° ATDC)Figure 13 - In-Cylinder Pressure Curves for High EGR Cases (-10° to 15° ATDC)and Figure 14 - HRR Plot for High EGR Cases (-5° to 20° ATDC)present the in-cylinder pressure and HRR for the high EGR cases. Under high EGR operation, the high CN fuels behave more distinctly from one another. This separation in behavior is particularly interesting for this study, and it was a goal in the development of this experiment.

The high CN fuels, FACE 5, the PME/FACE 1 blend, and the GTL/FACE 1 blend behave relatively similarly in their heat release and pressure rise profiles. The ignition delay for all fuels increases under the high EGR condition, which is a sign that combustion is being stressed for all fuels. Because of the increase in ignition delay for all of the fuels, the modes of combustion between the high and low CN fuels are more similar than under low EGR operation.

The peak heat release for each fuel is reduced by the introduction of the higher rate of EGR. This reduction in peak heat release drives down the in-cylinder temperatures achieved, which will greatly affect the emissions produced.

The chemical and physical differences between the fuels being tested becomes apparent under high EGR operation. Diesel #2, which is less controlled in its production, behaves differently under high EGR operation than the other fuels. This difference in behavior is due to a number of factors which are determined during the fuel production such as CN, viscosity, distillation temperature, aromatic content, and density. There is a slight difference in CN that will affect the performance between the 55 CN fuels, and the 51 CN Diesel #2. Fuel properties such as T90, aromatic content, and viscosity begin to play a larger role in the fuel's behavior under high EGR operation.

The low CN FACE 1 fuel exhibits a slight low temperature heat release (LTHR) from 1° to 3.5° ATDC under high EGR operation. This LTHR is not exhibited by any of the higher CN fuels under this load and EGR condition.

4.2. Engine Performance

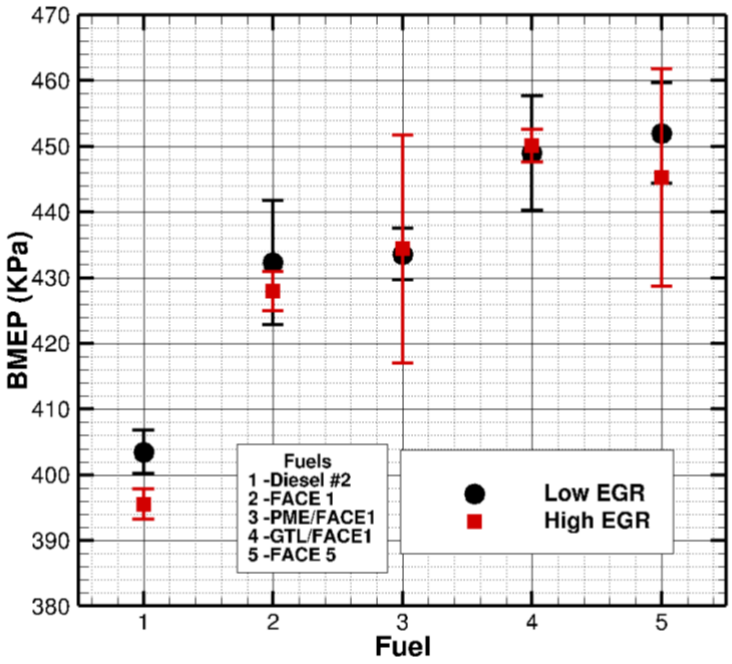

Figure 15 - Brake Mean Effective Pressure

Figure 15 - Brake Mean Effective Pressurepresents the BMEP produced by all fuels at high and low EGR. The BMEP produced across the fuel blends varied slightly. Of particular interest, the BMEP that was produced by Diesel #2 was substantially lower than the other fuels being tested. As mentioned in the experimental design section, the fuels do have slightly different energy densities and physical properties. The variances seen in the BMEP produced during testing are functions of these different properties. The resolution available in the control system did not allow for appropriate metering of fuel in order to ensure a constant flow of chemical energy into the cylinder. Because each fuel was tested at a constant injection pressure

and duration, the differences seen in the BMEP produced are directly related to the varying fuel properties including density, viscosity, energy density, T90, aromatic content, and CN.

The GTL/FACE 1 blend and FACE 5 produced a similar BMEP under the same operating conditions, and the PME/FACE 1 blend behaved more similarly to the low CN FACE 1 fuel. These differences in BMEP are due to slightly different energy densities of the fuels. From the properties of the base fuels, the PME/FACE 1 blend has lower energy density than the GTL/FACE 1 blend. Slight variances in BMEP were accepted in this experiment because the mass of fuel injected was held constant across all fuels.

The BMEP produced using this fueling strategy is different for each fuel due to differences in energy density and physical properties; however, the load conditions are appropriate for comparison because mass of fuel injected is held constant. Setting a constant BMEP across all fuels required extensive development testing that was not feasible with the fuel quantities available.

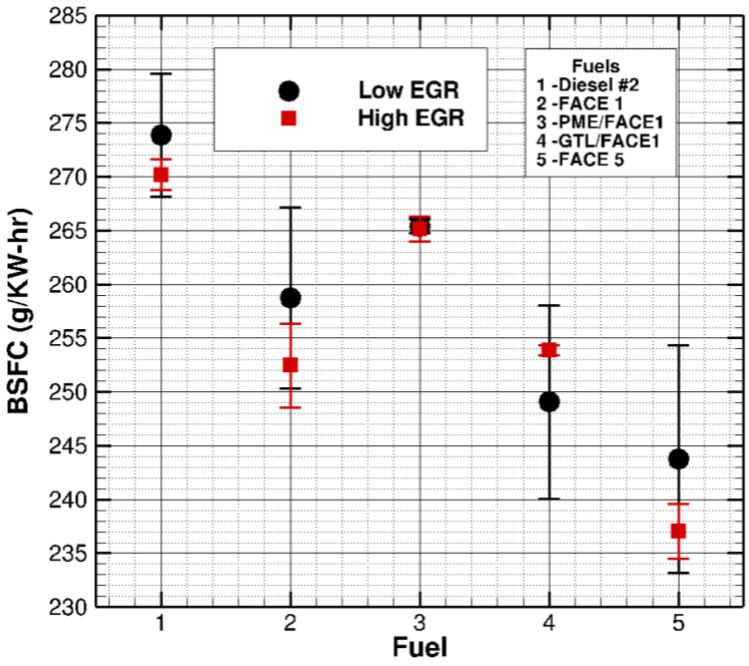

Figure 16 - Brake Specific Fuel Consumption

Following in line with the BMEP produced with each fuel, the BSFC for each fuel produced interesting results. Figure 16 - Brake Specific Fuel Consumptionpresents the BSFC for each fuel under high and low EGR operation. The BSFC for Diesel #2 was much higher than any of the other fuels under both high and low EGR operation. This difference in BSFC indicates that the fuel quality and purity of the FACE fuels and high CN blends enabled the engine achieve greater efficiency. The high CN FACE 5 exhibited better performance than the FACE 1 blends. Density effects will play a role in the fuels' behavior and BSFC performance. The PME/FACE 1 blend is denser, and slightly less energy dense than the other fuels, so it will have higher brake specific fuel consumption than the other high CN fuels. Due to the density effects and the lower energy content, the PME/FACE 1 fuel blend has higher BSFC than even the low CN FACE 1

fuel. With the exception of the GTL/FACE 1 fuel, each fuel's BSFC decreased with the increasing EGR; however, the PME/FACE 1 blend showed little to no sensitivity to increasing EGR.

The two neat FACE fuels have the same designed aromatic content and T90 distillation temperature, but the density, viscosity, and other physical properties are quite different. The viscosity and density differences will lead to slight differences in the total mass of fuel delivered to the cylinder during injection. The physical differences and the CN effect cause the high CN FACE 5 fuel to have lower BSFC than the low CN FACE 1 fuel.

The percentage deviation in BSFC from the standard high CN FACE 5 fuel is presented in Table 5:

Fuel	High EGR	Low EGR
Diesel #2	+13.98%	+12.35%
FACE 1	+6.51%	+6.16%
PME/FACE 1	+11.86%	+8.89%
GTL/FACE 1	+7.11%	+2.19%

Table 5 - BSFC Percentage Deviation from FACE 5

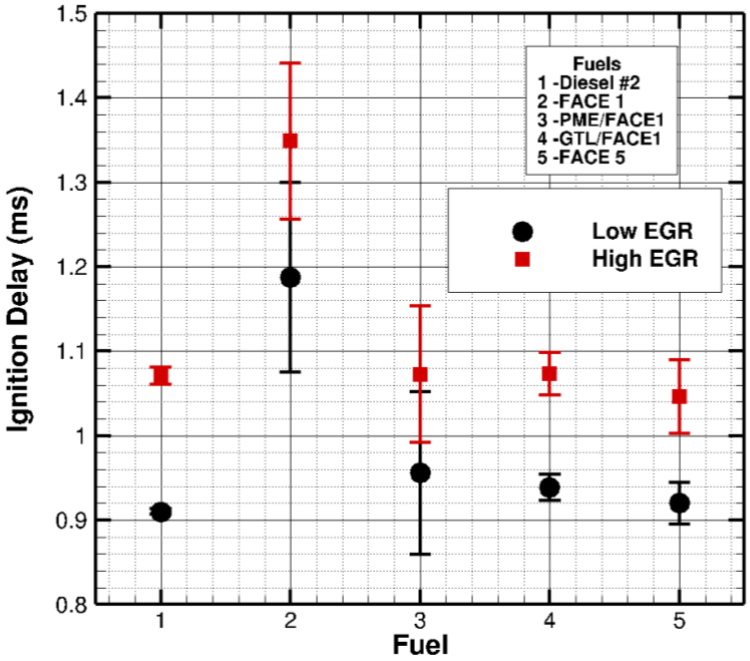

Figure 17 - Ignition Delay (ms) (SOI to 10% MFB)

Figure 17 - Ignition Delay (ms) (SOI to 10% MFB)and Figure 18 - Ignition Delay (CAD) (SOI to 10% MFB)present the ignition delay for each fuel in milliseconds and CAD. Ignition delay is most heavily driven by the CN of a fuel. The high CN fuels exhibit shorter ignition delays than the low CN FACE 1 fuel. Despite there being a CN difference between the baseline Diesel #2 fuel and the high CN neat FACE 5 and the blends, the ignition delay for Diesel #2 is comparable to the other high CN fuels. There is a slight difference in the ignition delays between the FACE 5 fuel and the GTL/FACE 1 and PME/FACE 1 fuel blends. Differences in the fuel chemistry and density can account for the small difference, and there are also likely to be slight non-linear blend effects in the fuel.

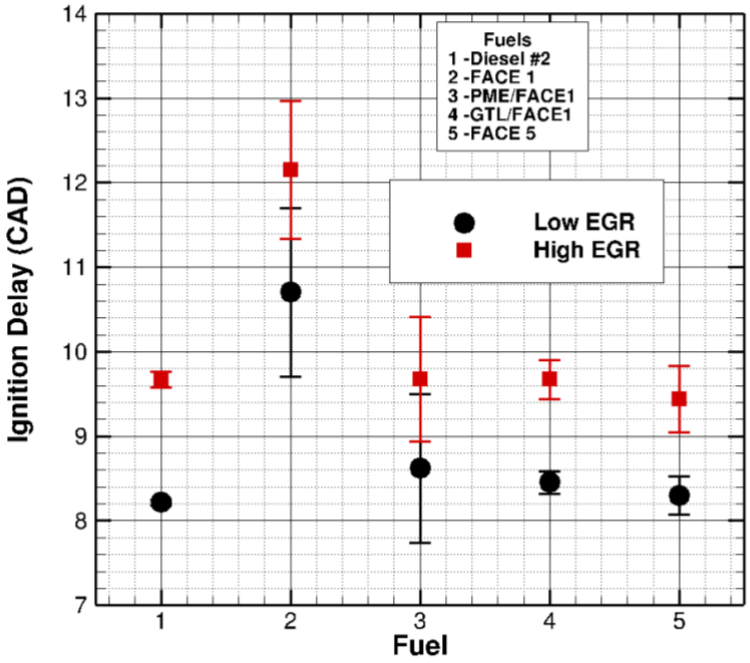

Figure 18 - Ignition Delay (CAD) (SOI to 10% MFB)

All of the fuels responded to the introduction of EGR similarly. The ignition delay data suggests that for all fuels, the ignition delay is increased by 12-18% when the EGR fraction is increased. This is due to the increased equivalence ratio in the cylinder, and the changing ratio of specific heats when the EGR diluent is introduced. The introduction of EGR also drives down the in-cylinder temperatures that the fuel experiences upon injection, which will lengthen the ignition delay of each fuel.

The ignition delay results show that blending the high CN PME and GTL fuels into the low CN FACE 1 fuel sufficiently increased the CN of the FACE 1 blends to match that of the high CN FACE 5 fuel. However, the efficiency and emissions data must be analyzed in order to appropriately gauge the effect of the fuels on the engine.

The percentage of deviation in ignition delay from the standard high CN FACE 5 fuel is presented in Table 6:

Fuel	High EGR	Low EGR
Diesel #2	+2.31%	-1.10%
FACE 1	+28.85%	+28.99%
PME/FACE 1	+2.49%	+3.87%
GTL/FACE 1	+2.57%	+1.99%

Table 6 - Ignition Delay Deviation from FACE 5

4.3. Engine Efficiency

The primary engine efficiencies that are of interest in this study are the brake fuel conversion efficiency (BFCE) and the combustion efficiency. The BFCE measures the engine's ability to convert the available chemical energy in the fuel into usable work. The BFCE takes into account differences in the fuel's energy content and density in order to evaluate the fuels on a level playing field. The combustion efficiency reports the level to which the fuel in the cylinder is fully oxidized.

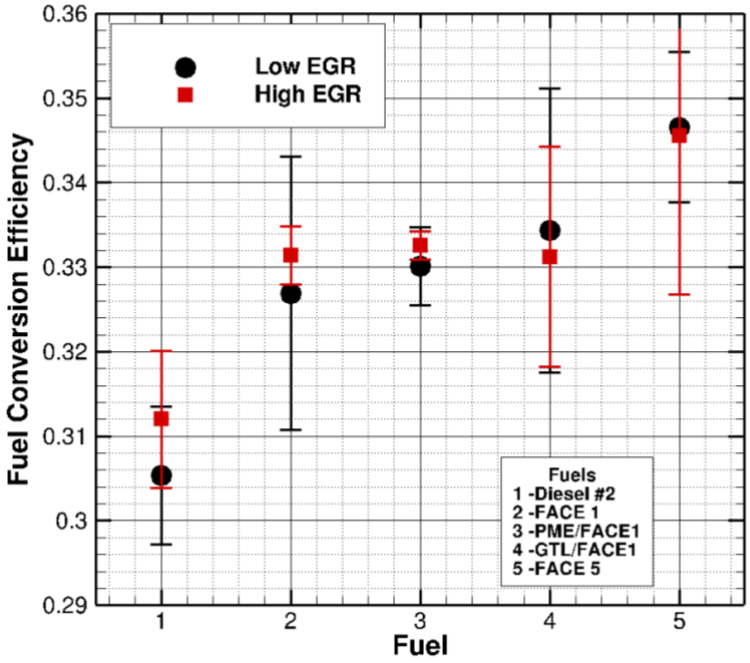

Figure 19 - Brake Fuel Conversion Efficiency

Figure 19 - Brake Fuel Conversion Efficiencypresents the BSFC for each fuel. The BFCE had little response to the CN of a specific fuel compared to the uncertainty associated with day-to-day ambient conditions. The Diesel #2 fuel provided the lowest BFCE of any of the test fuels, and the neat FACE 5 fuel had the highest BFCE. The fuels had very slight responses to the introduction of EGR, with the influence of EGR being the most apparent for Diesel #2 and the neat FACE 1 fuel. The neat FACE 5 and the GTL/FACE 1 blend produced reduced BFCE under high EGR operation.

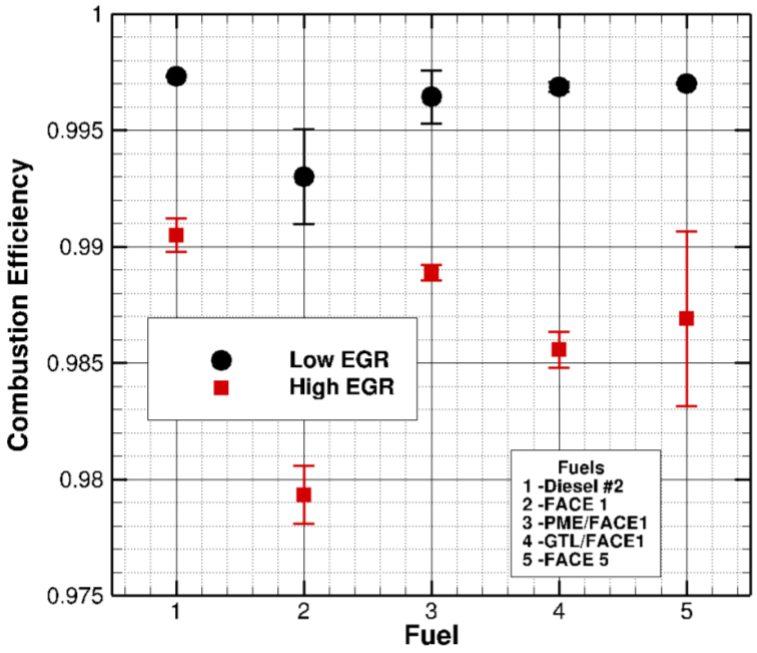

Figure 20 - Combustion Efficiency

Figure 20 - Combustion Efficiencypresents the combustion efficiency for each fuel. The fuel-lean nature of the operating conditions produce an in-cylinder environment in which very high levels of combustion efficiency can be achieved. The effects of increased CN can be seen in the combustion efficiency data. The neat FACE 1 fuel has lower combustion efficiency than the higher CN fuels. This reduction of combustion efficiency with reduced CN is due to the mode of combustion that occurs for the low CN fuel. Since the fuel spends more time pre-mixing in the cylinder, the burning is mainly pre-mixed, and there is less diffusion burning than what is seen for the high CN fuels. During pre-mixed burning, there may be pockets of fuel that do not fully combust, and the shorted diffusion burning period does not allow for combustion of the remaining fuel. The low CN fuel also has a shorter total burn time in the cylinder before the cylinder volume begins to expand. The balance between pre-mixed and diffusion burn that

occurs with the high CN fuels leads to more complete combustion. The high CN blends and the high CN FACE 5 fuel showed slightly more sensitivity to increasing EGR than the base Diesel #2. Increasing EGR tends to decrease combustion efficiency due to lower in-cylinder temperatures, and causing a richer equivalence ratio in the cylinder.

4.4. Emissions

4.4.1. Carbon Dioxide and Oxygen

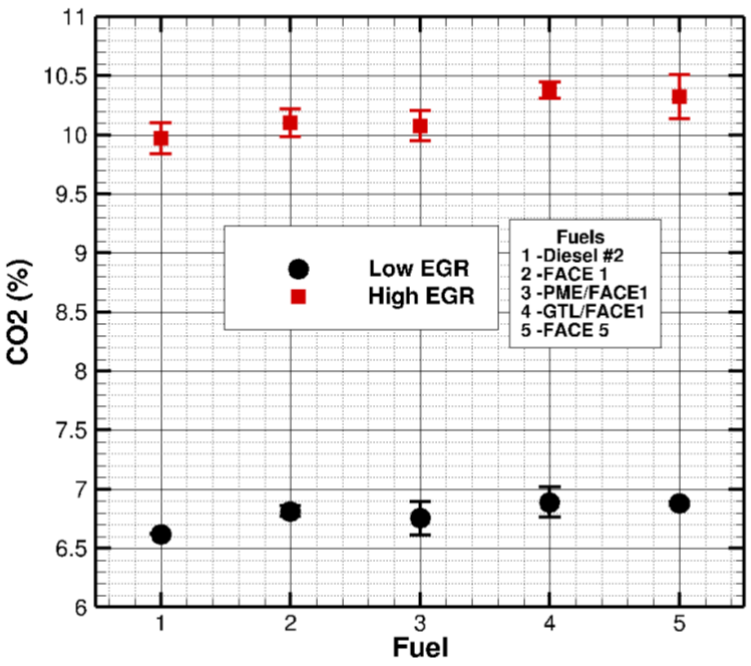

Figure 21 - CO2 Emissions

The CO_2 and O_2 emissions are largely unaffected by the changing fuel properties in this study. The primary driving force changing CO_2 and O_2 emissions percentages is the introduction of EGR. The CO_2 and O_2 emissions respond inversely to increasing EGR fraction.

Figure 21 - CO2 Emissionspresents the CO_2 emissions for each fuel. As EGR is increased, the CO_2 in the exhaust increases because the fresh charge being drawn into the cylinder during the intake stroke contains a much higher level of CO_2 than normal atmospheric air. Thus, the exhaust contains a percentage of CO_2 that is left over from the previous cycles. As EGR increases, the O_2 percentage in the exhaust decreases because less fresh charge of atmospheric air is being drawn into the cylinder. The intake of fresh atmospheric air is decreased from 90 kg/hr in low EGR operation to 60 kg/hr in high EGR operation. The fresh charge is also being diluted by the EGR that is being introduced into the intake manifold.

The fuels have slightly different oxygen content, which will cause there to be slightly different O2 percentages in the exhaust. Figure 22 - O2 Emissions presents the O2 emissions for each fuel. The PME fuel is an oxygenated biofuel, so it is expected that the PME/FACE 1 fuel will contain slightly higher levels of O2 in the exhaust [61]. Fuel flowrate differences between the fuels also can account for slightly higher O2 emissions while operating with Diesel #2, which has higher combustion efficiency.

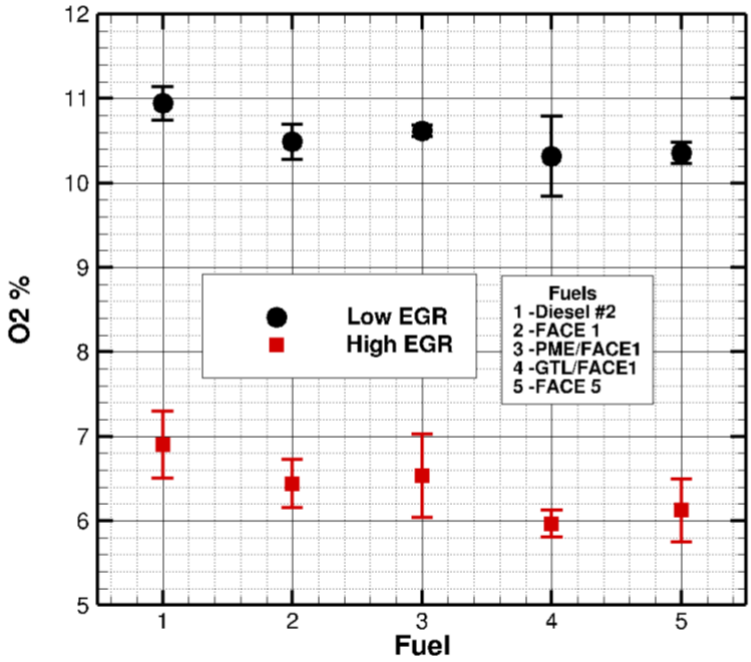

Figure 22 - O2 Emissions

4.4.2. Carbon Monoxide and Hydrocarbon

The CO and THC emissions are reported in Brake Specific terms in order to remove small variances in the power produced by the different fuels. CO and THC emissions plots in volume fraction [ppm] are available in the Appendix for reference.

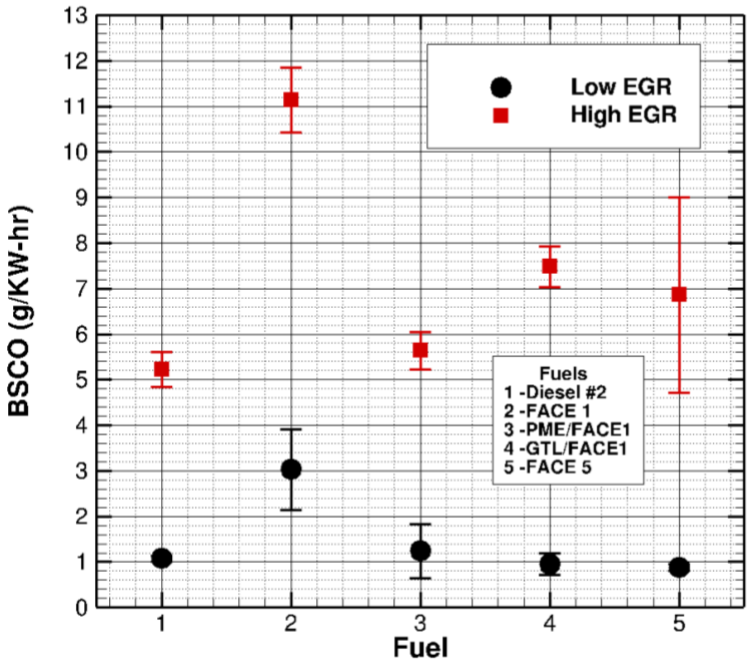

Figure 23 - Brake Specific CO Emissions (g/KW-hr)

Brake specific CO emissions are presented in Figure 23 - Brake Specific CO Emissions (g/KW-hr). CO emissions are heavily dependent on the combustion process that occurs in the cylinder. The CO production increases with increased EGR fraction for all fuels. The CN effect is very apparent in the CO emissions for the neat FACE 1 fuel under both high and low EGR operation. As the ignition delay increases for the FACE 1 fuel, the combustion becomes less efficient. The fuel does not fully oxidize to form CO_2, so additional CO is formed.

Despite the slightly lower CN, the Diesel #2 produced fewer CO emissions than the other fuels at high EGR operation, and the GLT/FACE 1 blend generated the highest levels of CO of the high CN fuels under high EGR operation.

The percentage deviation of BSCO from the standard high CN FACE 5 fuel is presented in Table 7:

Fuel	High EGR	Low EGR
Diesel #2	-23.88%	+21.72%
FACE 1	+62.27%	+243.60%
PME/FACE 1	-17.81%	+40.55%
GTL/FACE 1	+9.00%	+7.88%

Table 7 - BSCO Percentage Deviation from FACE 5

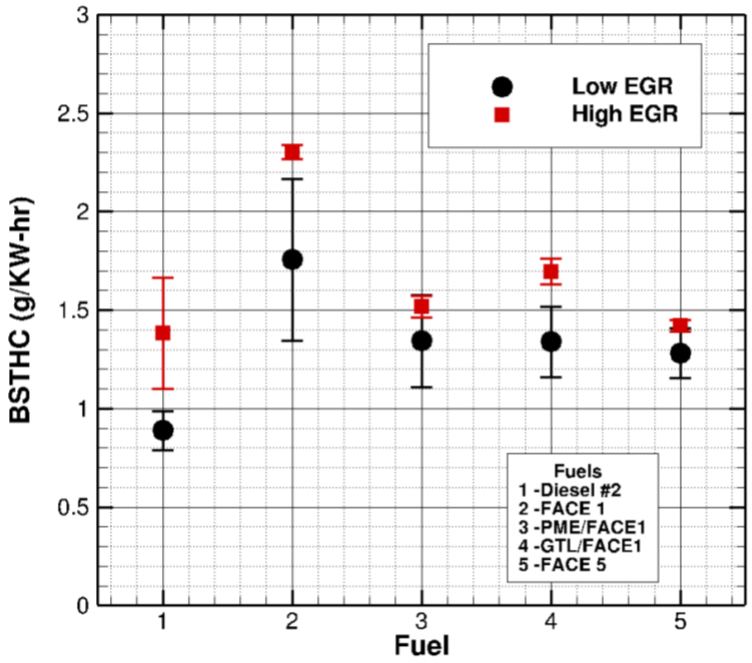

Figure 24 - Brake Specific THC Emissions (g/KW-hr)

Figure 24 - Brake Specific THC Emissions (g/KW-hr)presents the brake specific THC emissions. The THC emissions followed similar trends as the CO emissions. The THC emissions increased for each fuel with the introduction of high EGR. The low CN FACE 1 fuel produced the highest level of THC emissions of any fuel at any EGR level. Similar to the CO emissions, the GTL/FACE 1 blend produced higher THC emissions at high EGR than any of the other high CN fuels.

The percentage deviation of BSTHC from the standard high CN FACE 5 fuel is presented in Table 8.

Fuel	High EGR	Low EGR
Diesel #2	-2.81%	-30.76%
FACE 1	+62.09%	+37.01%
PME/FACE 1	+6.78%	+4.76%
GTL/FACE 1	+19.35%	+4.46%

Table 8 - BSTHC Percentage Deviation from FACE 5

4.4.3. Smoke Emissions

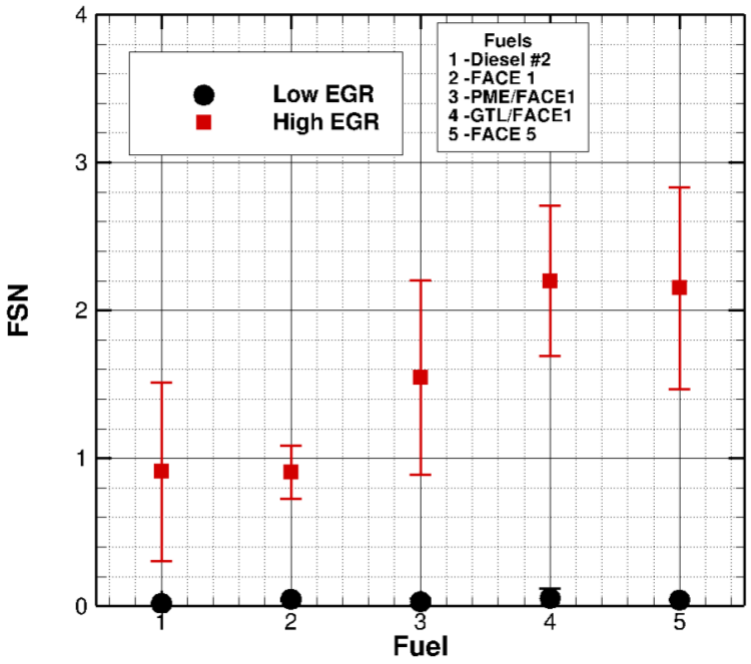

Figure 25 - Smoke Emissions (FSN)

Figure 25 - Smoke Emissions (FSN)presents the smoke emissions for each fuel. The smoke emissions follow expected trends in terms of the engine's response to increasing EGR. The smoke emissions are heavily dependent on the mode of combustion that occurs. For the high EGR case, the three high CN fuels exhibited a larger portion of diffusion burn during combustion. Virtually all smoke is formed in the diffusion burn portion of combustion [50].

The low CN FACE 1 fuel and Diesel #2 exhibited very similar pre-mixed burn profiles during high EGR operation, and each produced FSN values less than 1.0. Of the high CN fuels, the PME/FACE 1 blend produced the lowest amount of smoke emissions. The GTL/FACE 1 blend and the neat FACE 5 produced similar FSN values.

During low EGR operation, all of the fuels became sufficiently pre-mixed in order to facilitate near complete pre-mixed combustion and the high heat release leads to lower particulate formation. The engine produced very small FSN values (<0.1), and there was no appreciable difference in the FSN values produced by the different fuels.

The percentage deviation in FSN from the standard high CN FACE 5 fuel is presented in Table 9:

Fuel	High EGR	Low EGR
Diesel #2	-57.72%	-56.90%
FACE 1	-57.76%	+2.87%
PME/FACE 1	-28.11%	-35.06%
GTL/FACE 1	+2.33%	+20.11%

Table 9 - FSN Percentage Deviation from FACE 5

4.4.4. NOx Emissions

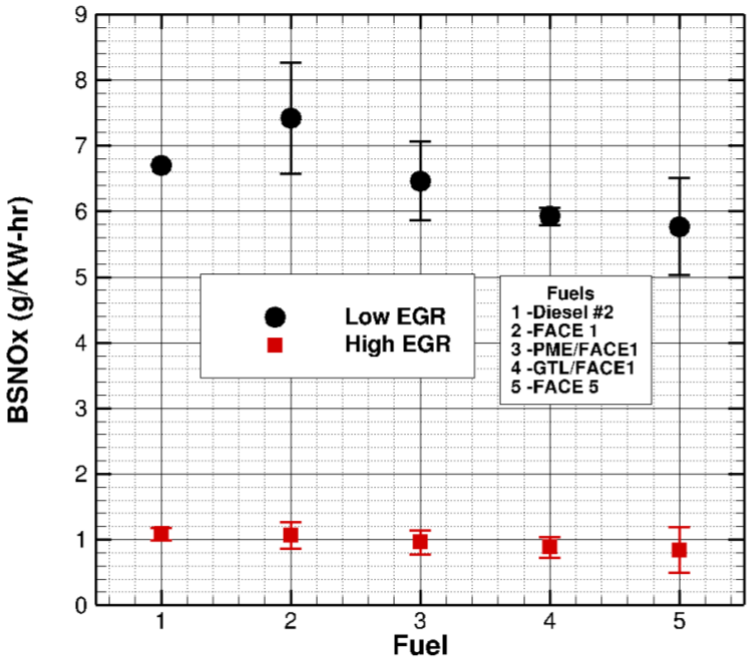

Figure 26 - Brake Specific NOx Emissions (g/KW-hr)

NOx emissions are presented in brake specific form in Figure 26 - Brake Specific NOx Emissions (g/KW-hr) in order to provide better clarity of the specific fuel effects. The NOx emissions in ppm concentration form are available in the Appendix.

The NOx emissions behave similarly for all high CN fuels under high EGR operation, with a slight decrease in NOx emissions occurring for the neat FACE 5 fuel and GTL/FACE 1 blend. The peak pressure that is generated, and the higher peak HRR for FACE 1 under high EGR operation leads to slightly higher levels of NOx formation than is seen for the high CN fuels.

Under low EGR operation, the differences in NOx formation between the fuels become more apparent. The low CN FACE 1 fuel produced the highest levels of NOx during low EGR operation. This high level of NOx is attributed to the longer ignition delay of the low CN fuel. The fuel has more time from the SOI to the point of ignition to mix with the air in the cylinder, thus leading to a very high level of pre-mixed combustion and high peak temperatures in the cylinder. The rapid burning of the low CN fuel causes NOx formation, and since the burn duration is shorter, the NOx does not break down during diffusion burning.

The GLT/FACE 1 blend and FACE 5 fuel produced the lowest levels of NOx emissions in the low EGR operation. While the PME/FACE 1 blend did perform better than the low CN FACE 1 fuel, it did not achieve the performance of the other high CN fuels. The percentage deviation of BSNOx from the standard high CN FACE 5 fuel is presented in Table 10:

Fuel	High EGR	Low EGR
Diesel #2	+28.63%	+16.18%
FACE 1	+26.18%	+28.55%
PME/FACE 1	+14.13%	+12.05%
GTL/FACE 1	+4.72%	+2.64%

Table 10 - BSNOx Percentage Deviation from FACE 5

5. CONCLUSIONS

The objective of this study was to assess the impacts on emissions and efficiency of altering fuel chemistry and physical properties while holding CN constant. with the exception of FSN under high EGR.

Utilizing a FAME biofuel such as PME, and a FT GTL diesel fuel as additives in lower CN diesel fuels has definite benefits in terms of efficiency and emissions. All emissions parameters with the exception of FSN were improved by implementing the higher CN fuel blends over the low CN FACE 1 fuel. The lower peak temperatures, and more complete combustion of the high CN fuels helped to reduce NOx, CO, and THC emissions.

The fuels did not; however, defeat the soot-NOx tradeoff. As the EGR fraction was increased, the smoke emissions increased for all fuels, and the high CN fuels experienced the largest increase in smoke emissions. The use of the PME/FACE 1 fuel blend provided the largest benefits in terms of smoke emissions under high EGR operation, while the GTL/FACE 1 fuel had the best efficiency and lowest NOx emissions of the blends under low EGR operation. Both the PME/FACE 1 fuel and the GTL/FACE 1 fuel produced lower smoke emissions under high EGR operation than the high CN FACE 5 fuel. The FACE 5 fuel did produce lower BSNOx emissions than any other fuel, and provided the greatest benefit in terms of fuel consumption and efficiency.

The HRR plots of the high and low EGR operation highlight the differences between the high and low CN fuels, with the low CN FACE 1 fuel experiencing nearly entirely pre-mixed combustion under high and low EGR, whereas the high CN fuels exhibited an increasing amount of pre-mixed burning as EGR was introduced.

Diesel fuel research is constantly evolving. Competing demands for fossil fuels and increasing regulations regarding emissions and efficiency have pushed further research and development in the field of diesel combustion. Alternative diesel fuels such as PME and GTL diesel have important roles to play in ensuring the long-term viability and usefulness of the diesel engine. As new techniques for improving the behavior of existing diesel fuel technologies are developed, there is an increasing importance being placed on the research being conducted to ensure compatibility with existing engines.

6. FUTURE WORK

The development and baseline testing that was conducted as a part of this study gleaned a large amount of information about the testing process and procedures that must be followed when conducting fuel research on the existing test apparatus. Future work should include developing processes and procedures that improve the reliability of data collection.

Future work should be conducted to compare the FACE fuels and the high CN FACE blends under different operating conditions and fueling strategies. In order to best characterize the differences between the fuel blends, a test matrix including higher load conditions should be devised. The fuels should also be tested in a multi-injection study to assess the effect of varying injection strategy on efficiency and emissions. The fuel blends should also be tested for their applicability in LTC techniques in order to defeat the soot-NOx trade-off.

Additional testing should be conducted using the high PME and GTL fuels as additives in conventional Diesel #2. The performance of Diesel #2 with regards to NOx and smoke may be improved by the addition of a small amount of the high CN fuels.

An additional study into the effects of CN on the specific emissions constituents would glean more information about the effects of each fuel on the emissions created.

REFERENCES

[1] S. L. Kokjohn, R. M. Hanson, D. Splitter, and R. Reitz, "Fuel reactivity controlled compression ignition (RCCI): a pathway to controlled high-efficiency clean combustion," *International Journal of Engine Research,* vol. 12, no. 3, pp. 209-226, 2011.

[2] J. B. Heywood, *Internal combustion engine fundamentals* (McGraw-Hill series in mechanical engineering). New York: McGraw-Hill, 1988, pp. xxix, 930 p., 2 p. of plates.

[3] N. Ladommatos, M. Parsi, and A. Knowles, "The effect of fuel cetane improver on diesel pollutant emissions," *Fuel,* vol. 75, no. 1, pp. 8-14, 1996.

[4] M. Hasegawa, Y. Sakurai, Y. Kobayashi, N. Oyama, M. Sekimoto, and H. Watanabe, "Effects of fuel properties (content of FAME or GtL) on diesel emissions under various driving modes," SAE Technical Paper0148-7191, 2007.

[5] T. Wu, Z. Huang, W.-g. Zhang, J.-h. Fang, and Q. Yin, "Physical and chemical properties of GTL− diesel fuel blends and their effects on performance and emissions of a multicylinder DI compression ignition engine," *Energy & Fuels,* vol. 21, no. 4, pp. 1908-1914, 2007.

[6] M. Oguma, S. Goto, K. Oyama, K. Sugiyama, and M. Mori, "The possibility of gas to liquid (GTL) as a fuel of direct injection diesel engine," SAE Technical Paper0148-7191, 2002.

[7] T. L. Alleman and R. L. McCormick, "Fischer-Tropsch diesel fuels-properties and exhaust emissions: A literature review," SAE Technical Paper0148-7191, 2003.

[8] P. Risberg, G. Kalghatgi, H.-E. Ångstrom, and F. Wåhlin, "Auto-ignition quality of diesel-like fuels in HCCI engines," SAE Technical Paper0148-7191, 2005.

[9] S. Kimura, O. Aoki, Y. Kitahara, and E. Aiyoshizawa, "Ultra-clean combustion technology combining a low-temperature and premixed combustion concept for meeting future emission standards," SAE Technical Paper0148-7191, 2001.

[10] T. J. Jacobs, S. V. Bohac, D. N. Assanis, and P. G. Szymkowicz, "Lean and rich premixed compression ignition combustion in a light-duty diesel engine," SAE Technical Paper0148-7191, 2005.

[11] T. Gallant *et al.*, "Fuels for advanced combustion engines research diesel fuels: analysis of physical and chemical properties," *SAE International Journal of Fuels and Lubricants,* vol. 2, no. 2009-01-2769, pp. 262-272, 2009.

[12] R. Diesel, "diesel," ed: Google Patents, 1895.

[13] K. Kitano, I. Sakata, and R. Clark, "Effects of GTL fuel properties on DI diesel combustion," SAE Technical Paper0148-7191, 2005.

[14] G. Knothe, "Biodiesel and renewable diesel: a comparison," *Progress in energy and combustion science,* vol. 36, no. 3, pp. 364-373, 2010.

[15] W. Cannella *et al.,* "Advanced alternative and renewable diesel fuels: detailed characterization of physical and chemical properties," *Coordinating Research Council, Alpharetta, GA,* 2013.

[16] J.-H. Ng, H. K. Ng, and S. Gan, "Characterisation of engine-out responses from a light-duty diesel engine fuelled with palm methyl ester (PME)," *Applied Energy,* vol. 90, no. 1, pp. 58-67, 2012.

[17] S. Bezergianni and A. Dimitriadis, "Comparison between different types of renewable diesel," *Renewable and Sustainable Energy Reviews,* vol. 21, pp. 110-116, 2013.

[18] M. Alnajjar *et al.,* "Chemical and physical properties of the fuels for advanced combustion engines (FACE) research diesel fuels," *CRC Report No. FACE-1,* 2010.

[19] J. Li, "Assessing Potential Differences of Diesel Fuel Effects on Combustion and Engine Behavior Betweeen Differently-Sized Engines," Mechanical Engineering, Texas A&M University, 2017.

[20] C. J. Mueller *et al.,* "Methodology for formulating diesel surrogate fuels with accurate compositional, ignition-quality, and volatility characteristics," *Energy & Fuels,* vol. 26, no. 6, pp. 3284-3303, 2012.

[21] C. J. Mueller *et al.,* "Diesel surrogate fuels for engine testing and chemical-kinetic modeling: Compositions and properties," *Energy & Fuels,* vol. 30, no. 2, pp. 1445-1461, 2016.

[22] J. Li, T. K. Bera, M. Parkes, and T. J. Jacobs, "A Study on the Effects of Cetane Number on the Energy Balance between Differently Sized Engines," SAE Technical Paper0148-7191, 2017.

[23] R. Westerholm and K.-E. Egebäck, "Exhaust emissions from light-and heavy-duty vehicles: chemical composition, impact of exhaust after treatment, and fuel parameters," *Environmental health perspectives,* vol. 102, no. Suppl 4, p. 13, 1994.

[24] A. S. f. Testing and Materials, "ASTM D975, Standard Specification for Diesel Fuel Oils," ed: ASTM International West Conshohocken, PA, 2011.

[25] M. J. Murphy, J. D. Taylor, and R. L. McCormick, *Compendium of experimental cetane number data*. National Renewable Energy Laboratory Golden, CO, 2004.

[26] D. L. Siebers, "Ignition delay characteristics of alternative diesel fuels: implications on cetane number," SAE Technical Paper0148-7191, 1985.

[27] T. W. Ryan, "Correlation of physical and chemical ignition delay to cetane number," SAE Technical Paper0148-7191, 1985.

[28] G. Bogin, A. M. Dean, M. A. Ratcliff, J. Luecke, and B. T. Zigler, "Expanding the experimental capabilities of the ignition quality tester for autoigniting fuels," *SAE International Journal of Fuels and Lubricants,* vol. 3, no. 2010-01-0741, pp. 353-367, 2010.

[29] G. Knothe, A. C. Matheaus, and T. W. Ryan III, "Cetane numbers of branched and straight-chain fatty esters determined in an ignition quality tester☆," *Fuel,* vol. 82, no. 8, pp. 971-975, 2003.

[30] B. T. Zigler, "Fuels for Advanced Combustion Engines," 2012.

[31] R. Ryskamp, G. Thompson, D. Carder, and J. Nuszkowski, "The Influence of High Reactivity Fuel Properties on Reactivity Controlled Compression Ignition Combustion," SAE Technical Paper0148-7191, 2017.

[32] V. Hosseini *et al.*, "Effects of cetane number, aromatic content and 90% distillation temperature on HCCI combustion of diesel fuels," SAE Technical Paper0148-7191, 2010.

[33] C. E. Dumitrescu, W. S. Neill, H. Guo, V. Hosseini, and W. L. Chippior, "Fuel property effects on PCCI combustion in a heavy-duty diesel engine," *Journal of Engineering for Gas Turbines and Power,* vol. 134, no. 5, p. 052801, 2012.

[34] W. De Ojeda, T. Bulicz, X. Han, M. Zheng, and F. Cornforth, "Impact of fuel properties on diesel low temperature combustion," *SAE International Journal of Engines,* vol. 4, no. 2011-01-0329, pp. 188-201, 2011.

[35] K. Anand, Y. Ra, R. Reitz, and B. Bunting, "Surrogate model development for fuels for advanced combustion engines," *Energy & Fuels,* vol. 25, no. 4, pp. 1474-1484, 2011.

[36] F. Ma and M. A. Hanna, "Biodiesel production: a review," *Bioresource technology,* vol. 70, no. 1, pp. 1-15, 1999.

[37] A. S. f. Testing and Materials, *Standard Specification for Biodiesel Fuel Blend Stock (B100) for Middle Distillate Fuels*. ASTM International, 2012.

[38] M. Lapuerta, O. Armas, and J. Rodriguez-Fernandez, "Effect of biodiesel fuels on diesel engine emissions," *Progress in energy and combustion science,* vol. 34, no. 2, pp. 198-223, 2008.

[39] M. H. M. Yasin, R. Mamat, K. Sharma, and A. F. Yusop, "Influence of palm methyl ester (PME) as an alternative fuel in multicylinder diesel engine," *Journal Mechanical Engineering and Sciences,* vol. 3, pp. 331-9, 2012.

[40] B. R. Moser, "Biodiesel production, properties, and feedstocks," *In Vitro Cellular & Developmental Biology-Plant,* vol. 45, no. 3, pp. 229-266, 2009.

[41] K. S. Tyson and R. L. McCormick, *Biodiesel handling and use guidelines*. US Department of Energy, Energy Efficiency and Renewable Energy, 2006.

[42] A. Steynberg, "Introduction to fischer-tropsch technology," *Studies in surface science and catalysis,* vol. 152, pp. 1-63, 2004.

[43] M. E. Dry, "The fischer–tropsch process: 1950–2000," *Catalysis today,* vol. 71, no. 3, pp. 227-241, 2002.

[44] R. H. Clark, I. Lampreia, R. J. Stradling, and M. Schmidt, "Emissions performance of shell GTL fuel in the context of future fuel specifications," SAE Technical Paper0148-7191, 2006.

[45] S. G. Solutions, "GTL Fuel Knowledge Guide," vol. 2, ed.

[46] K. Kitano, S. Misawa, M. Mori, I. Sakata, and R. H. Clark, "GTL fuel impact on DI diesel emissions," SAE Technical Paper0148-7191, 2007.

[47] T. Kroeger, "Reducing the Emissions and Efficiency Penalties of Low Temperature Combustion through Low Heat Rejection Operation," Master of Science, Mechanical Engineering, Texas A&M University, 2017.

[48] M. Patterson, S.-C. Kong, G. Hampson, and R. D. Reitz, "Modeling the effects of fuel injection characteristics on diesel engine soot and NOx emissions," SAE Technical Paper0148-7191, 1994.

[49] G. A. Ban-Weiss, J. Chen, B. A. Buchholz, and R. W. Dibble, "A numerical investigation into the anomalous slight NO x increase when burning biodiesel; a new (old) theory," *Fuel processing technology,* vol. 88, no. 7, pp. 659-667, 2007.

[50] D. R. Tree and K. I. Svensson, "Soot processes in compression ignition engines," *Progress in Energy and Combustion Science,* vol. 33, no. 3, pp. 272-309, 2007.

[51] O. I. Smith, "Fundamentals of soot formation in flames with application to diesel engine particulate emissions," *Progress in Energy and Combustion Science,* vol. 7, no. 4, pp. 275-291, 1981.

[52] H. Song, B. Tompkins, J. Bittle, and T. Jacobs, "Comparisons of NO emissions and soot concentrations from biodiesel-fuelled diesel engine," *Fuel,* vol. 96, pp. 446-453, 2012.

[53] K. K. Takeda, Hideki, "Downsizing and Modular Configuration of Analyzers," in "Motor Exhaust Gas Analyzer MEXA-7000 Series," 1995.

[54] H. I. Incorporated, "Instruction Manual for CLA-220 Chemiluminescent Analyzer," ed. Irvine, California, 1995.

[55] H. I. Incorporated, "Instruction Manual FMA-220/FIA-220/MPA-220," ed, 1990.

[56] H. I. Incorporated, "Instruction Manual AIA-210/220 Infrared Analyzer," ed. Irvine, California, 1995.

[57] M. Navas, A. Jiménez, and G. Galan, "Air analysis: determination of nitrogen compounds by chemiluminescence," *Atmospheric Environment,* vol. 31, no. 21, pp. 3603-3608, 1997.

[58] S. Ali and J. Walker, "Measurement of gas concentrations (O2, CO2, N2O and volatile agents)," *Anaesthesia & Intensive Care Medicine,* vol. 15, no. 11, pp. 526-529, 2014.

[59] J. P. Szybist and B. G. Bunting, "Cetane number and engine speed effects on diesel HCCI performance and emissions," SAE Technical Paper0148-7191, 2005.

[60] A. J. Wheeler and A. R. Ganji, *Introduction to engineering experimentation*. Prentice Hall Englewood Cliffs, NJ, 1996.

[61] F. Wu, J. Wang, W. Chen, and S. Shuai, "A study on emission performance of a diesel engine fueled with five typical methyl ester biodiesels," *Atmospheric Environment,* vol. 43, no. 7, pp. 1481-1485, 2009.

APPENDIX

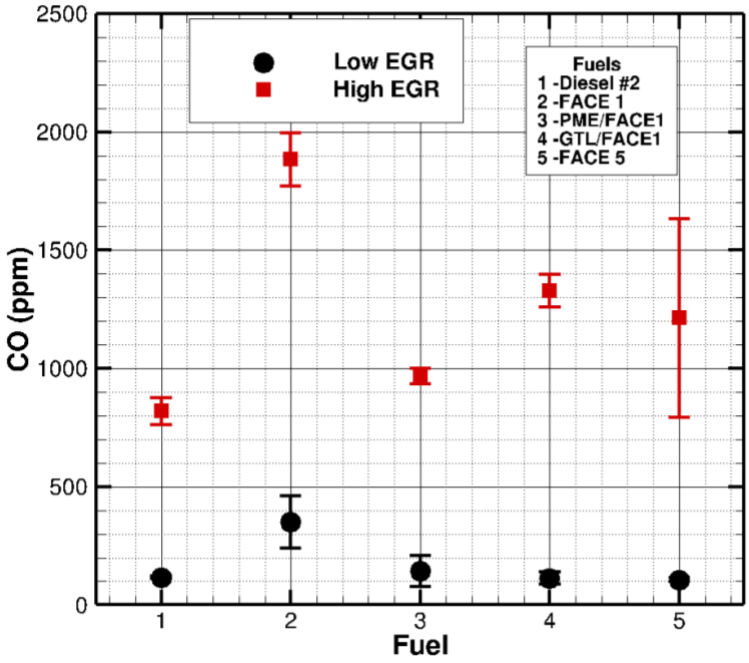

Figure 27 - CO Emissions (ppm)

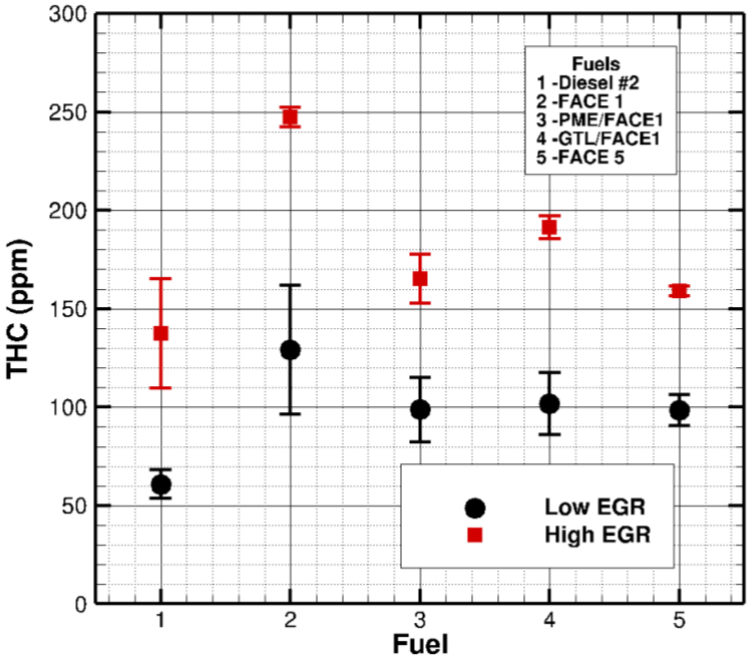

Figure 28 - THC Emissions (ppm)

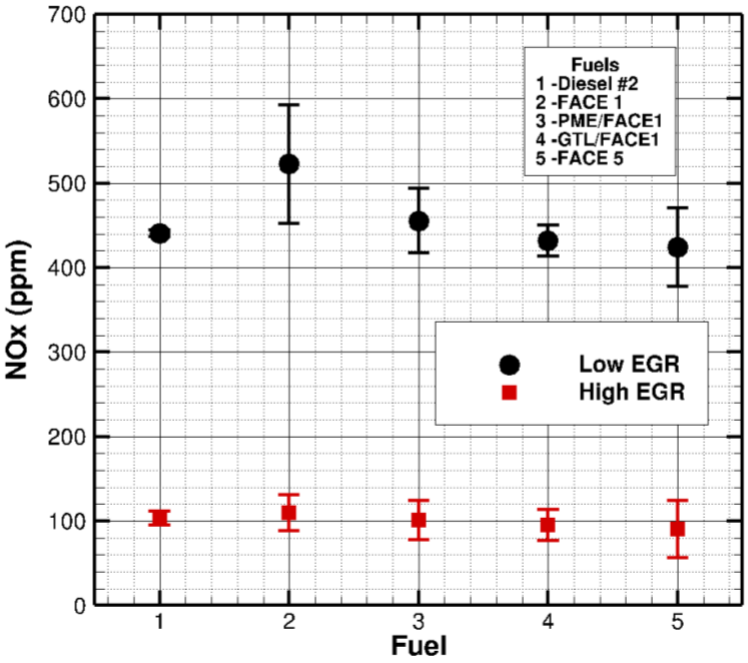

Figure 29 - NOx Emissions (ppm)